A143 Investigation of 2D-LC/QTOF/MS for the Detection of Illicit Drugs

Yuriy Uvaydov, MS, 99 Tenth Avenue, Ste 721, New York, NY 10011*

After attending this presentation, attendees will gain an understanding of Two-Dimensional Liquid Chromatography (2D-LC) technique coupled with Quadrupole Time-Of-Flight Mass Spectrometry (QTOF/MS). The attendees will understand how the technique can potentially be applied to resolving complex mixtures of forensically relevant samples in a single analysis.

This presentation will impact the forensic science community by discussing how the technique can be used to enhance data quality, allowing for an increased chromatographic peak capacity and sensitivity for complex sample matrices. The findings and methodology can provide forensic laboratories with the ability to identify alternative means for the detection and identification of seized drugs.

The majority of cases encountered by forensic chemists are analyzed utilizing traditional methodologies such as Gas Chromatography/Mass Spectrometry (GC/MS), Gas Chromatograph-Flame Ionization Detector (GC/FID), Fourier Transform Infrared-Attenuated Total Reflectance (FTIR-ATR), and Liquid Chromatography/Mass Spectrometry (LC/MS). The use of LC/QTOF/MS has gained popularity in recent years for its use in targeted screening as well as characterization of unknown designer drugs. LC/QTOF/MS has a superior advantage over traditional methodologies as it can deliver accurate mass determination and provide highly specific mass-to-charge spectral data, with accuracies spanning in the milli-Dalton range for parent and fragment ions. As such, routine and targeted-based methods may be set up that are fully automated for screening and identification purposes. By integrating a second-dimension aspect to chromatography, the capabilities of the LC/QTOF/MS may further be enhanced, particularly for isobaric compounds or other designer drugs that are similar in structure, sharing some of the same chemical properties used to achieve chromatographic separation.

In order to investigate the suitability of 2D-LC/QTOF/MS for identification of seized drugs, experiments have been performed to assess operational characteristics in the analysis of 15 beta-ketone derivatives of amphetamine, commonly known as designer cathinones. The goal of this study was to assess the function of 2D-LC using an orthogonal combination of stationary phases, different mobile phase compositions, isobaric compounds, and limits of detection. The method employed an Agilent® 1200 binary pump with a Hydrophilic Interaction Liquid Chromatography (HILIC) column, coupled to an Agilent® 1290 Infinity Ultra High-Pressure Liquid Chromatography (UHPLC) (via a six-port valve) with a ZORBAX® Extend C18 column. TOF/MS full-scan spectra were acquired in positive Electrospray Ionization (ESI) mode over 50-1000m/z scan range using reference masses m/z 121.0509 and 922.0098. Additional TOF MS parameters were set as follows: fragmentor voltage at 150V; capillary voltage at 4,000V; skimmer voltage at 65V; nebulizer pressure at 50psi; gas temperature at 350°C; gas flow rate at 13L/min. Collision Induced Dissociation (CID) of precursor ions were obtained in targeted MS/MS mode using a collision cell with nitrogen as a collision gas.

Illicit Drugs, QTOF, 2D-LC

 ** Presenting Author*