K20 Qualitative Screening of Multiple Designer Drug Classes Using Polymer-Based SPE and LC/QTOF/MS

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After attending this presentation, attendees will understand the advantages and limitations of using high-resolution Tandem Mass Spectrometry (MS/MS) for screening of designer drugs from multiple classes. Attendees will also learn about the advantages of using polymeric solid phase extraction cartridges for screening of designer drugs. In addition, the presentation with demonstrate the applicability of a high-resolution MS/MS screening method in combination with a previously created high-resolution MS/MS spectral library.

This presentation will impact the forensic science community by providing a high-resolution MS/MS method using a polymer-based solid phase extraction cartridge to qualitatively screen for more than 200 designer drugs from classes including cathinones, indanes, phenethylamines, piperazines, tryptamines, and synthetic cannabinoids.

Designer drugs are compounds that are used in an attempt to evade current drug laws. Many of these compounds are structurally or pharmacologically similar to common illegal drugs of abuse. In the past few years, there has been an increase of recreational designer drug use among users. In an effort to combat designer drug use, the U.S. government permanently scheduled 26 designer drugs in the Synthetic Drug Abuse Prevention Act of 2012. Due to potential dangers and legal implications that arise from the use of such drugs, it is critically important that forensic toxicology laboratories have the capability to screen and detect as many designer drugs as possible in a single specimen.

In order to address the dynamic nature of designer drug use and to screen for these drugs effectively, many laboratories have turned to mass spectrometric screening techniques. Liquid Chromatography/Quadrupole Time-Of-Flight/Mass Spectrometry (LC/QTOF/MS) was used for this project because it enables the analyst to have higher confidence when identifying a compound, due to its high resolution, high mass accuracy, and MS/MS capabilities. The LC/QTOF/MS also has high sensitivity in full-scan mode, which is useful for screening designer drugs. This project focused on creating and validating a screening method that employs a Bond Elut® Plexa™ PCX Solid-Phase Extraction (SPE) cartridge, which is a polymer-based cation mixed-mode cartridge and an Agilent® 6530 Accurate-Mass QTOF LC/MS. The solid phase extraction method for this project was created after optimizing the load, wash, and elution steps in order to achieve the highest percent recovery of the designer drugs. Different volumes of sample and wash/elution steps were investigated to determine which volumes would produce the lowest Limit Of Detection (LOD) while minimizing the interferences that may be present in the post-extraction solution. The LC gradient, auto MS/MS parameters, and library search parameters were optimized to produce a method that generated the lowest amount of false positives while also avoiding false negatives. Once the method was optimized, it was then validated using Scientific Working Group for Forensic Toxicology (SWGTOX) recommendations. The LOD for most of the designer drugs was <10ng/mL. No significant carryover or interference was observed. Ionization suppression and enhancement fell in the acceptable range (±25%).

The results demonstrated that the use of a polymer-based SPE cartridge and high-resolution LC/QTOF/MS instrumentation can be useful tools in comprehensive screening for designer drugs. The larger binding capacity of the polymer-based SPE cartridge combined with the high resolution of the LC/QTOF/MS enables higher confidence in drug identification when screening for designer drugs. While there are limitations to this screening method, i.e., some isobaric and poorly ignitable compounds in Electrospray Ionization (ESI) mode, the method represents a new, useful tool for the detection of designer drugs in human matrices.

Designer Drugs, LC/QTOF/MS, SPE

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