B129 High-Throughput Screening of Drugs of Abuse Using a Robust Thermal Extraction Ionization Source (TEIS)

Pierre Negri, PhD, SCIEX, Redwood City, CA 94065; Oscar G. Cabrices, PhD, SCIEX, Redwood City, CA 94065; Neil Davenport, SCIEX, Centre Park, Warrington UK WA1 1RX, UNITED KINGDOM; Ashley Sage, SCIEX, Centre Park, Warrington UK WA1 1RX, UNITED KINGDOM; Peter Luke, Mass Spec Analytical, Bristol UK BS34 7RP, UNITED KINGDOM; Carl Fletcher, Mass Spec Analytical, Bristol UK BS34 7RP, UNITED KINGDOM*

Learning Overview: The objective of this study is to demonstrate the high level of sensitivity and robustness of this combined system for rapid and confident compound identification of drugs of abuse.

Impact on the Forensic Science Community: The abuse of opioids and other related drugs continue to pose serious public health and safety issues worldwide As these substances continue to cause widespread intoxications resulting in fatalities worldwide, robust and comprehensive detection is critical to enable forensic laboratories to rapidly and accurately identify these substances. This presentation will impact the forensic science community by describing a method combining a TEIS coupled with a Mass Spectrometry (MS) system used for ultra-fast screening of drugs of abuse without the need for chromatography or extensive sample preparation. The combined system can quickly identify unknown drugs of abuse with a high level of confidence suitable for rapid forensic screening.

Methods: The TEIS was combined to an MS system for the identification of drugs of abuse. Upon integration of the source to the mass spectrometer, the source was heated to 285°C to volatilize the solvent injection, and a sample pump was used to draw the gaseous molecules toward the ionization region. Samples were injected via a microliter syringe into an injection port at the front of the top block for liquid standards or a slot between the two heated blocks for paper swabs. MS detection was performed in positive mode using a multiple reaction monitoring scheme to detect precursor and product ions of each of the targeted analytes.

Results: The use of the TEIS on a mass spectrometer enabled the rapid acquisition of MS data for high-throughput screening. First, drug-of-abuse standards were injected into the source and MS parameters were tuned. This process was used for each of the drug-of-abuse standards to determine the fragmentation pattern of each analyte and to appropriately select two product ions. Drug-of-abuse residues were tested by swiping a piece of paper on a dry surface onto which an unknown drug-of-abuse mixture was left to dry. The piece of paper was then inserted into two heated blocks of the TEIS and positive identification of the unknown drugs of abuse was accomplished by monitoring the thermal desorption profile in the form of an Extracted Ion Chromatogram (XIC) for two transitions monitored for each drug analyte. This process enabled the confident detection and quantitation of cocaine, amphetamine, and MDMA as the unknown compounds in the swab residue. Quantification of the drug residues present on a cell phone screen was also performed. The amount of the drug residues transferred to the paper swab was calculated using the area value for each of the XIC peaks resulting from the thermal desorption profile for each of the two transitions and solving for x using the linear regression equation. Using this method, the averaged values for cocaine, amphetamine, and MDMA were found to be 8.16 ng, 7.84 ng, and 5.53ng, respectively.

Conclusion/Discussion: Accurate identification and confident identification of low levels of drug residues is feasible using the extracted XICs based on the MRM transitions for the drug analytes. This demonstrates that the combination of Atmospheric Pressure Chemical Ionization (APCI) with thermal desorption is suitable as a fast sampling and screening method for trace analysis of drug residues. This approach shows potential application for trace analysis of drug residues from containers and parcels for high throughput security screening.

Drugs of Abuse, Mass Spectrometry, High-Throughput Detection

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*Presenting Author