K27 Drug Screening Using a High Resolution Accurate Mass System

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The goal of this presentation is to show the use of fast, high resolution, accurate mass system capable of generating TOF-MS data with up to 20 product ion spectra in under a second.

This presentation will impact the forensic science community by giving attendees a great option for generating high resolution, accurate mass data for use in forensics and toxicology.

Objectives: This research evaluates the use of a fast, high resolution, accurate mass system capable of generating TOF-MS data with information dependent acquisition (IDA) of up to 20 TOF-MS/MS in one second for drug screening purposes. Initial drug identification was accomplished by accurate mass MS and confirmation by accurate mass product ion spectrum which was searched against a library. The use of an existing product ion spectra library generated on a hybrid triple quadrupole ion trap system with the data generated from high resolution, accurate mass system is also evaluated.

Methods and Sample Preparation: Blood samples (250µL) were precipitated with the addition of 750µL of acetonitrile. Samples were then vortexed, centrifuged and the supernatant evaporated, before reconstitution with 500µL of 10/90 acetonitrile/water. Urine samples were diluted with five volumes of 10/90 acetonitrile/water.

Chromatography: The separation was carried out on a PFP Propyl 50mm x 2.1mm x 5µ column. Mobile phase A consisted of 0.2% formic acid and 2mM ammonium formate in water and mobile phase B consisted of 0.2% formic acid and 2mM ammonium formate in acetonitrile. A linear gradient starting at 10% organic and ending at 90% organic was used with a total flow rate of 0.7mL/min and a total run time of 17.5 min.

Mass Spectrometer: The drug screening method consisted of a full range TOF-MS survey scan with IDA-triggering of up to 20 accurate mass product ion scans. Total cycle time for the TOF-MS – IDA – TOF-MS/MS (20) was approximately one second. The product ions were automatically searched against an existing library containing spectra for over 1200 compounds. The library was previously generated on a hybrid triple quadruple ion trap system and was evaluated for compatibility with the accurate mass system.

Results and Conclusion: Positive blood and urine samples, as well as spiked matrix samples, were used for the evaluation of the drug screening method and the library search tool along with the library previously generated on a different mass spectrometer. All compounds in the spiked matrix samples were correctly identified and confirmed. High concentrations of antidepressants, pain medications, or drugs of abuse were observed in the positive samples. The method allows for the positive identification of over 1,200 drugs and metabolites by using accurate mass along with MS2 confirmation. With the fast, high resolution, accurate mass system, TOF-MS along with 20 product ion scans were collected in about one second allowing for more analytes to be confirmed even with multiple co-eluting analytes. TOF-MS scan allowed for identification of analytes by exact mass with mass error less than 5ppm. Confirmation was accomplished by searching all generated product ion scans against a library with more than 1,200 compounds generated on the hybrid triple quadruple ion trap system. Library search scores ranged between 75% and 98% showing that even though the library was generated on a different mass spectrometer, the spectra can be used since similar fragmentation patterns are obtained in both instruments.

Accurate Mass, Mass Spectrometry, TOF-MS