

K12 A Novel Method to Extend the Detection Window of Drug Administration in Victims of Malignant Assault With Hybrid LC/MS/MS Technology Combining Triple Quadrupole and Ion Trap Technology

Andre Schreiber, PhD*, Applied Biosystems/MDS Sciex, 71 Four Valley Drive, Concord, Ontario L4K4V8, Canada

After attending this presentation, attendees will understand the advantages of using hybrid triple quadrupole linear ion trap mass spectrometry to identify phase I and phase II metabolites of drugs.

This presentation will impact the forensic community and/or humanity by helping to determine whether a drug has been administered, even after the parent drug has been completely eliminated from the victim's body.

A research method has been developed to detect drug intake long after a dose has been administered. This is achieved by detecting specific Phase I and Phase II metabolites that are continually excreted post dose, far longer than the parent drug. Drugs and metabolites are detected in positive mode utilizing specific Multiple Reaction Monitoring (MRM) experiments. Informationdependent criteria for acquisition of an enhanced product ion (EPI) scan result in precursor ion fragmentation to characteristic product ions. Fragmentation occurs at varying collision energies and enables spectral comparison to drug libraries. In addition, Phase II metabolites, namely glucuronides are detected using true Neutral Loss (NL) scanning and identified by EPI acquisition and spectral matching. The loss of dehydroglucuronic acid with a m/z ratio of 176 is characteristic of all glucuronide metabolites. Chromatographic separation is based on a 2.1 mm ID, 5 micron Gemini column with an acetonitrile, formic acid, and ammonium formate mobile phase gradient ramp optimized for separation of various drugs and metabolites. The method is used to detect drugs in forensic and clinical research samples and was developed to provide greater scope, sensitivity, and selectivity compared to conventional methods of drug detection. The method will help to determine whether or not a drug has been taken/administered even after the parent drug has been completely eliminated from the body of the victim.

LC/MS/MS, Metabolites, Toxicology