



K48 Screening for Drugs and Metabolites in Hair Specimens by LC/TOF/MS

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After attending this presentation, attendees will gain knowledge about the contribution of hair as a matrix for the detection of drugs using Liquid Chromatography Time-of-Flight Mass Spectrometry (LC/TOF/MS) and how these results compare to those previously reported for other postmortem biological matrices originating from the same decedent.

This presentation will impact the forensic science community by establishing a procedure for the screening of drugs and metabolites in hair by LC/TOF/MS and recognizing hair as a valuable alternative matrix for drug screening when blood and urine sample collection is delayed or unavailable within the detectable window for those matrices.

The mechanism by which drugs are incorporated into hair has been most simply modeled as passive diffusion into the rapidly growing cells of the hair follicle; however, alternative studies describe mechanisms for incorporation that occur post-formation of the hair shaft that may be drug-dependent. Taken together, forensic analyses largely benefit from the very stable matrix that the interior of the hair shaft provides, thus allowing for a detection window that is days to years post-exposure. To this end, several studies have described methodologies for the analysis of hair, most recently utilizing the specificity and data range accomplished with time-of-flight mass spectrometry.

Because of advances in technology and affordability, LC/TOF/MS has gained increasing popularity as a screening tool for its ability to determine mass measurements that are accurate to several decimal places (rather than the nominal or unit mass measurements of ± 0.01 Da) coupled with the creation of a target drug compound list with retention time data which allows for rapid, selective, specific, and retrograde screening of target compounds. To this end, this study's laboratory has recently validated an LC/TOF/MS screening method and has created an Accurate-Mass Retention-Time (AMRT) Personal Compound Database Library for more than 100 pure reference standard drug compounds routinely and newly encountered in forensic toxicology examinations.

This study describes the procedure developed in the laboratory for the analysis of drugs extracted from hair by LC/TOF/MS. Postmortem head hair samples were collected from a variety of medicolegal cases for which chronic drug use had been documented, and forensic analyses on blood, urine, and other routine toxicology specimens from the same case had been completed by the laboratory. This presentation will highlight five interesting cases involving scene information and toxicology findings in blood, hair, and other specimens. Approximately 10mg from the total hair sample was subjected to a decontamination/wash step with a solution of 0.1% Triton™ X-100, and subsequently extracted with an extraction buffer composed of 200mM dithiothreitol with gentle rocking at room temperature for two hours. The final external wash and internal extracts were combined with internal standard, filtered, and analyzed using LC/TOF/MS to scan for the presence of prescription, illicit, and newer designer drugs.

Separations were performed using an Agilent® Eclipse Plus C18 1.8um, 3.0 x 100mm column. The chromatography conditions were able to resolve isomers such as codeine and hydrocodone, but could not differentiate between 3,4-methylenedioxy-methamphetamine (MDMA) and methedrone. In the case of overlapping isomers, supportive information was obtained from distinguishing accurate mass measurements of associated metabolites. The mass analyzer was an Agilent® 6230 TOF/MS operated in positive ion scan mode with mass scanning from 100 to 1,000m/z.

This presentation will discuss the significant strengths and weaknesses of this technique in comparison to traditional methods of analysis. However, this type of comprehensive toxicology analysis will extend the abilities of laboratory operations and provide more interpretive information for the forensic toxicologist. The analytes discovered in hair could also reveal a medicinal history that would be useful to a pathologist in classifying death when very little else is known or proven.

Hair Analysis, LC/TOF/MS, Drugs of Abuse