

## W2 Advanced Mass Spectrometry (MS) Techniques for Forensic Analysis: What Does the Future Hold?

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After attending this presentation, attendees will be better able to evaluate and select advanced MS techniques for solving various analytical problems in forensic science, including identification of unknowns, rapid throughput approaches to forensic sample preparation, novel ionization, and fragmentation approaches in hyphenated mass spectrometric techniques.

This presentation will impact the forensic science community by introducing attendees to some of the most recent advances in MS technology and their potential application to solve challenges in forensic investigations. This workshop has a strong interdisciplinary focus.

Advances in MS technology over the past decade profoundly affect the way forensic toxicologists and drug chemists approach screening of samples for the presence of controlled substances and other drugs. Immunoassay and Gas Chromatography/Mass Spectrometry (GC/MS) analysis, once considered the "gold standard" for initial detection and exclusion of specific drugs/drug classes, are being replaced by Liquid Chromatography/Mass Spectrometry (LC/MS) and Liquid Chromatography/Tandem Mass Spectrometry (LC/MS/MS) methods due to increased availability of new instrumentation and performance improvements in existing technologies. An overview of the application of MS to drug screening in a modern toxicology laboratory, illustrated with casework data, will be provided. Topics will include the reasons behind the trend toward LC/MS analysis, comparison of the advantages of different MS technologies, different models for sample screening, and the use and limitations of high resolution and accurate mass data.

Multiplexing is a high-throughput solution which allows minimization of MS idle time by using two High-Performance Liquid Chromatography (HPLC) systems configured to one detector. This technique allows overlap of chromatographic runs while collecting spectrometric data in predefined windows. Two HPLC systems also permit simultaneous analysis by two methods employing different mobile phase systems. A 2D LC/MS/MS system increases sample throughput while preserving equilibration time.

Stable Isotope Ratio Mass Spectroscopy (IRMS) has been used in geochemistry and other fields for decades. Since the introduction of Gas Chromatography/Combustion IRMS (GC/C/IRMS), Compound-Specific Isotope Analysis (CSIA) has become increasingly utilized to determine isotopic composition in various fields. Several forensic applications of CSIA have been documented, including: determination of illicit drug preparations, identification of counterfeit pharmaceuticals, determination of doping in sports, and investigation of ignitable liquids and explosives; however, GC/C/IRMS is not without challenges. Labor-intense sample preparation, poor sensitivity, delicate instrumentation, and lack of uniform standards are difficulties which have hindered widespread adoption. This presentation will introduce attendees to GC/C/IRMS and detail current forensic GC/C/IRMS applications, with a focus on sports-doping steroid analysis. Present state-of-the-art and future possibilities of the methodology will be presented.

Several technologies for rapid and/or on-site MS have migrated from prototype instruments in research laboratories to fully validated commercial systems. Unreliability of color tests for preliminary identification of emerging synthetic drugs have increased interest in this instrumentation in forensic science. Additionally, fieldable MS has been used extensively in battlefield forensics for on-site identification of drugs and explosives. Currently, fieldable mass spectrometers can be used for preliminary identification and in the near future, these instruments could be used for rapid definitive identification in the field. Coupling simplified sampling strategies such as ambient ionization, solid phase microextraction, and thermal desorption have been key to success with these instruments. An overview of currently available instrumentation, primarily GC/MS and ion-traps, and their implementation by forensic scientists will be presented as well as a discussion of emerging instrumentation.

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## Workshop - 2016

In the final presentation, attendees will be left with some thought-provoking ideas of where the discipline of forensic MS is headed in the future. From the days of Gas Chromatography/Flame Ionization Detector (GC/FID) use as a confirmatory approach to the current uses of LC/MS/MS and higher resolution options, the forensic science community has adapted to changes in the analytical technologies and implemented them to address challenges in casework. Technology will continue to advance and provide new opportunities for addressing challenges in our everyday work. This presentation will outline anticipated changes that will occur in the forensic drug and toxicology communities over the coming years.

Mass Spectrometry, Sample Preparation, Advanced Techniques

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