K53 Comparison of Various Liquid Chromatography–Mass Spectrometry Technologies for the Analysis of Forensic Toxicology Samples for Commonly Encountered Drugs

H. Chip Walls, BS, University of Miami, Department of Pathology, Forensic Toxicology Laboratory, 12500 SW 152nd Street, Building B, Miami, FL 33177; Peter R. Stout, PhD*, and Jeri D. Ropero-Miller, PhD*, RTI International, 3040 Cornwallis Road, PO Box 12194, Building 3, Room 116, Research Triangle Park, NC 27709; and John M. Hughes, PhD, Agilent Technologies, 6612 Owens Drive, Pleasanton, CA 94588; and Michael Zumwalt, PhD, Agilent Technologies, 9780 South Meridian Boulevard, Englewood, CO 80112*

After attending this presentation participants will have a greater under- standing of how a variety of mass spectral technologies may be applicable to particular analytical challenges.

This presentation will impact the forensic science community conducting analysis of "drugs" by providing comparative data from a variety of mass spectral techniques on the same samples.

Introduction: A wide array of mass spectral and hyphenated mass spectral technologies is currently available for analysis of small molecules. It has become increasingly confusing for investigators to understand which technologies may be best for particular analytical applications. Specifically, this presentation will provide an overview of LC/QqQ (triple quad), LC/QTOF (time of flight), LC/TOF, LC/MS (single quad), LC/MS ion trap and DART-TOF (Direct Analysis in Real Time, Time of Flight MS) technologies. These technologies will be applied to the same samples to allow for the comparison of what types of technologies are advantageous for which types of applications. Samples will include postmortem specimens and DUID specimens.

Method: Typical forensic samples, blood from death and DUID cases, were prepared in sufficient amounts such that the same extracts could be analyzed on the various fragmentation and detection instruments. Samples were extracted in a manner appropriate for the matrix and suitable for the various ionization methods. For DART analysis, blood samples were intro- duced without sample preparation and with the same sample preparation as for LC/MS. Samples were run on an AccuTOF-DART system located at RTI International and on LC/MS systems located at the University of Miami forensic toxicology laboratory and at various Agilent application laboratories.

Results: Representative chromatograms and mass spectra will be presented. The various strengths and limitations of quadrupole-based technologies for quantification and SRM/MRM identification will be compared with identification of compounds using accurate mass and MSn techniques. The presentation will also discuss how individual technologies can accommodate both identification and quantification. Specifically, the different mass spectrometers will be discussed in light of each instrument's strengths and weaknesses for providing forensically-acceptable, highly sensitive screening and identification results.

Conclusions: These comparative MS/MS data provide examples appropriate to the challenges faced in forensic toxicology and demonstrate what various instruments are able to achieve. This presentation will provide examples from a variety of mass spectral technologies from at least two manufacturers and will hopefully provide the groundwork for further comparative studies to include upcoming technologies and more manufacturers.

Analytical Toxicology, Postmortem Toxicology, LC/MS

 ** Presenting Author*