Foreword

Presentations

Posters

Resources

Call for Abstracts

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FORENSIC SCIENCE EDUCATION

Virtual/Online Symposium: Current Trends In Forensic Toxicology

MAY 22–24, 2018

Remain Current on Critical Issues Facing Forensic Toxicologists Today!
Novel Psychoactive Substances (NPS)… The opioid crisis… Fentanyl/Carfentanil… Screening, identification, and confirmation… Workflow simplification. Learn from some of the world's leading forensic toxicologists about these critical topics and the various ways in which the related issues are being addressed. This inaugural virtual symposium provides you with ready access to some of today's leading researchers and practitioners without ever having to leave the laboratory.

Foreword
Presentations
Posters
Resources
Call for Abstracts

FOREWORD

It is my great pleasure to welcome you to this inaugural virtual symposium, Current Trends in Forensic Toxicology. Nearly 1,000 forensic toxicologists from all over the world attended the live event May 22–24, 2018. The event continues to make an impact through the recorded presentations, uploaded posters, and other resources that are now accessible through the links available in this e-book.

It is not surprising that the symposium was such an overwhelming success because the source of its inspiration was you and other members of the global forensic toxicology community. Throughout my travels, I have enjoyed conversations with many of you who have shared similar sentiments. Some of these conversations included feedback about common hurdles as well as opportunities for improvement related to live events:

- The challenge of attending meetings and conferences due to cost constraints and travel limitations
- The inability to leave the laboratory for extended periods because of continually increasing caseloads
- The lack of time allotted for oral platforms and follow-up questions at live conferences
- The lack of face-to-face meetings in certain geographic areas
- The challenge of sharing ideas and experiences across geographic borders, especially in places like Southeast Asia and Australia

You were the inspiration for this landmark event in which technology brought together members of the global forensic toxicology community. Thanks to members like you, virtual attendees enjoyed live interactions and the subsequent sharing of information without ever having to leave their computers. I hope that this event represents the beginning of a new era of global interaction as we seek to leverage new, more advanced technologies. We want these technologies to enable activities such as expert panel discussions with live audience participation and virtual poster sessions that allow you to interact live, one-on-one with different presenters.

If you are interested in speaking at this event in the future, please see the call for abstracts that appears on page 22 of this e-book. I hope you find the following resources useful and informative. And it is my sincere hope that you will join us live at next year's event tentatively scheduled for May 2019.

Warm regards,

Thomas J. Gluodenis, Jr., MFS, PhD

WW Forensic Industry Manager

Agilent Technologies

Thomas J. Gluodenis, Jr., MFS, PhD

Special thanks to:

This event would not have been possible without the efforts of many individuals. In particular, I want to thank

- Vasanthi Arjavalingam of Agilent Technologies for her tireless efforts and extreme attention to detail;
- Erica Fornaro of RTI International for her unwavering support;
- Josh Vickers (also of RTI) who served as a tireless advocate of this project, a consummate professional as a moderator, and an invaluable technical resource;
- Mike Baylor, formerly of RTI and now a forensic toxicology consultant, who suggested an accompanying poster session.

And last, but certainly not least, I want to thank our esteemed speakers who represent the very best that the forensic toxicology community has to offer: Dr. Simon Elliott, Dr. Sarah Kerrigan, Dr. Madeleine Swortwood, Dr. Stefan Toennes, Dr. Alexander van Nuijs, Dr. Robert Kronstrand, Dr. Dong-Liang Lin, and Dr. Ray H. Liu. My deepest gratitude to you all and to the many others who made this event a success.

Foreword

Presentations

Day 1–Tuesday

1. The Use of QTOF in Forensic Toxicology
   Simon Elliott, PhD
2. Evolving Methodologies Amenable to the Analysis of Drugs in Postmortem Specimens
   Dong-Liang Lin, PhD, and Ray H. Liu, PhD

Day 2–Wednesday

Day 3–Thursday

Posters

Resources

Call for Abstracts

PRESENTATIONS

Day 1

1. The Use of QTOF in Forensic Toxicology

VIEW RECORDING

ANNOTATED SLIDES

Simon Elliott, PhD, Director of Global Forensics, Alere Forensics (now Abbott), Malvern, United Kingdom

Abstract: The use of high-resolution mass-spectrometry (e.g., QTOF) has increased significantly in recent years as it provides an impressive number of advantages to analytical toxicology. These include the ability to perform general screening with identification of unknown compounds coupled with retrospective re-interrogation of results if new information comes to light. Targeted analysis can also be performed based on accurate mass detection and QTOF has particular advantages in the detection of more challenging analytes, such as Novel Psychoactive Substances (including synthetic cannabinoids and cathinones) and drug glucuronides. The latter enables longer windows of detection and confirmation of drug use through metabolite identification. QTOF also allows quantitation of compounds. This presentation will discuss the various advantages as well as the important considerations in implementing high-resolution mass-spectrometry in forensic toxicology. These include, identification parameters, detection window interpretation, deuterated internal standards, and isobaric/isomeric compounds.

Detailed Learning Objectives:

- Understand how QTOF may be used for general screening, including identification of unknown compounds.
- Understand how QTOF may be used for Novel Psychoactive Substance analysis.
- Understand the considerations of implementing QTOF in forensic toxicology.

Presentation PDF: https://mp634935.cdn.mediaplatform.com/634935/wc/mp/predeploy/cf/_cfdb14b1-20cc-b48e-c4d4-a79219795c8f_/Forensic-toxicology-symposium-day1-speaker1-pp-agilent.pdf

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Archival Registration: https://forensicrti.org/course/virtual-online-symposium-current-trends-in-forensic-toxicology-agilent/

Simon Elliott, PhD, Director of Global Forensics, Abbott (formerly Alere Forensics), Malvern, United Kingdom

Dr. Simon Elliott has more than 20 years' experience in forensic toxicology and is a Consultant Forensic Toxicologist and Director of Global Forensics at Abbott (formerly Alere Forensics). He was formerly the founder and Managing Director of Alere Forensics (formerly ROAR Forensics) in Malvern, Worcestershire, 2008–2017. He previously worked as a Clinical Scientist in the NHS at Birmingham City Hospital for more than 10 years; he was specifically involved in clinical and forensic toxicology as Section Head of Forensic Toxicology. He is Vice Chair of the United Kingdom and Ireland Association of Forensic Toxicologists (UKIAFT) and an executive board member of The International Association of Forensic Toxicologists (TIAFT).

Simon Elliott, PhD

Foreword

Presentations

Day 1–Tuesday

1. The Use of QTOF in Forensic Toxicology
   Simon Elliott, PhD
2. Evolving Methodologies Amenable to the Analysis of Drugs in Postmortem Specimens
   Dong-Liang Lin, PhD, and Ray H. Liu, PhD

Day 2–Wednesday

Day 3–Thursday

Posters

Resources

Call for Abstracts

PRESENTATIONS

2. Evolving Methodologies Amenable to the Analysis of Drugs in Postmortem Specimens

Dong-Liang Lin, PhD, Chief Forensic Toxicologist, Department of Forensic Toxicology, Institute of Forensic Medicine, Ministry of Justice, New Taipei City, Taiwan

Ray H. Liu, PhD, Professor Emeritus, Department of Criminal Justice, University of Alabama at Birmingham, Birmingham, Alabama; Editor-in-Chief, Forensic Science Review, Vancouver, Washington, USA

VIEW RECORDING

ANNOTATED SLIDES

Abstract: The organizational structure and function of the Institute of Forensic Medicine in Taiwan is similar to major medical examiner offices in the United States. The institute serves the entire country of 23 million. During the recent years, the Toxicology Department received postmortem specimens from slightly over 4,000 cases/year. This laboratory has keenly observed advances in the field of forensic toxicology and actively engaged in developing/adopting new methodologies to constantly increase the laboratory's effectiveness. This laboratory's adoptions of evolving methodologies (e.g., preliminary screen, sample preparation, and confirmation/quantitation) amenable to the analysis of drugs are the main focus of this presentation. Data derived from the analysis of drugs in urine specimens serve as the basis to illustrate how new approaches were developed/adopted. Merits of new methodologies are emphasized. For example, the newly adopted UHPLC-QTOF/MS approach enables simultaneous screen of all drugs that were included in the database (established in-house), with significantly higher detection rates over LC-IT/MS- and GC/MS-based methodologies. On the other hand, a LC-QQQ/MS-based methodology can confirm and quantitate many more drugs/metabolites (such as opioids, amphetamines, ketamine, benzodiazepines, barbiturates, and Novel Psychoactive Substances) in a single analytical run without the derivatization step.

Detailed Learning Objectives:

- Appreciate advances of preliminary screen, sample preparation, and confirmation/quantitation methodologies in forensic toxicology during the last 2 decades.
- Familiarize with the merits of UHPLC-QTOF/MS as a preliminary screen methodology in forensic toxicology.
- Recognize potential applications of QuEChERS approaches for sample preparation in forensic toxicology.
- Realize the merits of LC-QQQ/MS as a confirmation/quantitation methodology in forensic toxicology.

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Foreword

Presentations

Day 1–Tuesday

1. The Use of QTOF in Forensic Toxicology
   Simon Elliott, PhD
2. Evolving Methodologies Amenable to the Analysis of Drugs in Postmortem Specimens
   Dong-Liang Lin, PhD, and Ray H. Liu, PhD

Day 2–Wednesday

Day 3–Thursday

Posters

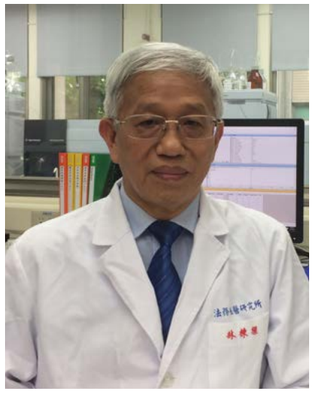
Resources

Call for Abstracts

PRESENTATIONS

Dong-Liang Lin, PhD, Chief Forensic Toxicologist, Department of Forensic Toxicology, Institute of Forensic Medicine, Ministry of Justice, New Taipei City, Taiwan

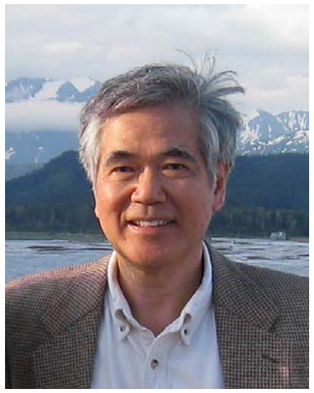
Dr. Dong-Liang Lin received a PhD in pharmacy from Taipei Medical University (Taipei, Taiwan); he received postmortem toxicology training in Cook County (Chicago, Illinois) and New Jersey State (Newark, New Jersey) Medical Examiner's Offices in the U.S. Dr. Lin joined the Institute of Forensic Medicine (IFM) in 2001 and currently serves as the Chief Toxicologist of the Institute's Forensic Toxicology Department. Prior to joining IFM, Dr. Lin worked for the Ministry of Justice's Bureau of Investigation laboratory (1987–2001) and received training in the U.S. Fish and Wildlife Service Forensics Laboratory (Ashland, Oregon). Dr. Lin has been actively working on analytical method development and has published more than 40 articles in peer-reviewed journals. Dr. Lin is a member of the American Academy of Forensic Sciences and The International Association of Forensic Toxicologists (TIAFT). He is also a member of the Taiwan Society of Forensic Medicine and the Taiwan Academy of Forensic Sciences.



Dong-Liang Lin, PhD

Ray H. Liu, PhD, Professor Emeritus, Department of Criminal Justice, University of Alabama at Birmingham, Birmingham, Alabama; Editor-in-Chief, Forensic Science Review, Vancouver, Washington

With a law degree from a police academy (now Central Police University) in Taiwan, Dr. Ray H. Liu received his PhD in chemistry from Southern Illinois University (Carbondale, Illinois). Dr. Liu has held positions at the University of Illinois at Chicago (Chicago, Illinois), U.S. Environmental Protection Agency's Central Regional Laboratory (Chicago), U.S. Department of Agriculture's Eastern Regional Research Center (Philadelphia, Pennsylvania), and Southern Regional Research Center (New Orleans, Louisiana). He was a faculty member at the University of Alabama at Birmingham (UAB) for 20 years, serving as the Director of UAB's Graduate Program in Forensic Science for the last 10 years. He retired in 2004 and was granted "professor emeritus" status in 2005. Following his retirement from UAB, Dr. Liu taught at Fooyin University (Kaohsiung, Taiwan) for 8 years (2004–2012). Dr. Liu's work has been mainly in the analytical aspects of drugs of abuse (criminalistics and toxicology), with a significant number of publications in each of the following subject matters: Enantiomeric analysis, quantitative determination using isotopic analogs as internal standards, correlation of immunoassay and GC-MS test results, specimen source differentiation, and analytical method development. Dr. Liu has authored/edited (or coauthored/coedited) several books, book chapters, and more than 120 articles in refereed journals. He is now the Editor-In Chief of Forensic Science Review and an editorial board member of several journals.



Ray H. Liu, PhD

PRESENTATIONS

Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

1. Coping with Requirements in Forensic Toxicology: Combination of Routine Laboratory and Forensic Science
   Prof. Stefan W. Toennes, PhD
2. LC/MS/MS Approaches for Identifying Emerging NPS
   Sarah Kerrigan, PhD, and Madeleine Swortwood, PhD

Day 3–Thursday

Posters

Resources

Call for Abstracts

Day 2

1. Coping with Requirements in Forensic Toxicology: Combination of Routine Laboratory and Forensic Science

VIEW RECORDING

ANNOTATED SLIDES

Prof. Stefan W. Toennes, PhD, Institute of Legal Medicine, Frankfurt/Main, Germany

Abstract: Forensic toxicology consists of specialized analytic procedures in the first place, but it also needs evidence-based toxicologic evaluation. Analytics on a contemporary level requires high sensitivities for the detection of low concentrations of modern medical and abused drugs. This typically means targeted analyses with liquid chromatography coupled to mass spectrometry (LC/MS/MS), which is not available unlimited in most labs. Therefore, to cope with the needs, the typically limited financial resources must be optimized (e.g., by using diversified equipment like GC-MS, GC-MS/MS and time-of-flight mass spectrometry [TOF]). In the forensic lab of Frankfurt/Main, Germany, the principal strategy is to use an LC/MS/MS targeted screening in all cases with the extension of untargeted screening and quantification by LC/TOF MS. Tandem mass spectrometry provides sufficient identification, while for a single-stage TOF MS (from our experience), the All-Ions approach may provide identifying fragments but not at very low concentrations and the huge data file sizes prohibit routine use. In our laboratory, the use of a GC-MS/MS in CI mode with two injectors and LTM (low thermal mass) columns substitutes for sensitive and fast LC/MS/MS (e.g., in the applications to determine cannabinoids in serum and EtG in hair).

However, forensic toxicology does not only consist of analytics, but also of forensic expertise. This requires continuing education of technical staff and toxicologists, but also practical experience (e.g., by participating in or initiating research projects). Data from controlled studies, especially with human subjects, give a personal impression of intra- and inter-individual variations, which is essential for forensic toxicological expertise.

For example, data on effects of "new psychoactive substances" are lacking due to their largely unknown toxicological properties. As a first attempt, a controlled study with the rather long-known synthetic cannabinoid JWH-018 was performed in which six subjects received 2- and 3-milligram doses as well as placebo via inhalation of pure substance in a blinded manner. The low doses produced only small effects but the "subjective high" was elevated and deficits in the critical tracking task and divided attention task were significant. Serum pharmacokinetics covered a time range of 12 hours and JWH-018 and five of its metabolites exhibited multi-exponential elimination similar to that of tetrahydrocannabinol (THC). The prominent decrease during the first hour after inhalation suggests a marked distribution, which could be the basis of prolonged excretion. This could already be deduced from residual JWH-018 and metabolites in serum and urine 3–4 weeks later. In the oral fluid (OF) samples obtained an hour or later after inhalation, concentrations were similar to serum with a median OF/S ratio of 1.4 (0.05–554) but with shorter detectability. In urine, the parent compound was not detectable, but 13 conjugated metabolites were detectable. The predominant metabolite was JWH-018 pentanoic acid with concentrations less than 5 nanograms/milliliter (ng/ml); other major metabolites were 5- and 4-HOpentyl-JWH-018, a hydroxy-keto metabolite and JWH-073 butanoic acid. The different excretion of carboxylic acid and hydroxylated metabolites may aid in evaluation of time of use. Further studies (e.g., with increased doses) are in progress.

In conclusion, to keep up with modern forensic toxicology requirements, diversified analytical equipment must be accompanied by the respective expertise, which can be gained by initiating and participating in scientific studies.

Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

1. Coping with Requirements in Forensic Toxicology: Combination of Routine Laboratory and Forensic Science
   Prof. Stefan W. Toennes, PhD
2. LC/MS/MS Approaches for Identifying Emerging NPS
   Sarah Kerrigan, PhD, and Madeleine Swortwood, PhD

Day 3–Thursday

Posters

Resources

Call for Abstracts

PRESENTATIONS

Detailed Learning Objectives:

- Know how to cope with typical analytical tasks in forensic toxicology with a combination of LC/MS/MS, GC-MS/MS, GC-MS and LC-TOF MS.
- Know how to perform analysis of cannabinoids in serum and ethyl glucuronide in hair with one GC-MS/MS device.
- Know about metabolites and pharmacokinetics of JWH-018 in serum, oral fluid, and urine.

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Archival Registration: https://forensicrti.org/course/virtual-online-symposium-current-trends-in-forensic-toxicology-agilent/

Prof. Stefan W. Toennes, PhD, Institute of Legal Medicine, Frankfurt/Main, Germany

Prof. Dr. Stefan Toennes was born in 1966. After studying pharmacy and working in the Institute of Experimental and Clinical Toxicology in Homburg/Saar, Germany, he graduated with his PhD in 1997. After habilitation in forensic toxicology in 2005, he was appointed extraordinary professor of Goethe University Frankfurt, Germany, and leads its Forensic Toxicology Department. He is member of several scientific committees and currently President of the German Society of Toxicological and Forensic Chemistry.

Prof. Stefan W. Toennes, PhD

Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

1. Coping with Requirements in Forensic Toxicology: Combination of Routine Laboratory and Forensic Science
   Prof. Stefan W. Toennes, PhD
2. LC/MS/MS Approaches for Identifying Emerging NPS
   Sarah Kerrigan, PhD, and Madeleine Swortwood, PhD

Day 3–Thursday

Posters

Resources

Call for Abstracts

PRESENTATIONS

2. LC/MS/MS Approaches for Identifying Emerging NPS

Sarah Kerrigan, PhD, Professor and Chair, Department of Forensic Science, Sam Houston State University, Huntsville, Texas

Madeleine Swortwood, PhD, Assistant Professor, Department of Forensic Science, Sam Houston State University, Huntsville, Texas

VIEW RECORDING

Dr. Sarah Kerrigan

ANNOTATED SLIDES

Dr. Madeleine Swortwood

ANNOTATED SLIDES

Abstract: With the rapid expansion of NPS and the increased presence of LC/MS/MS in forensic toxicology laboratories, validated analytical methodologies are necessary for screening and quantification of various NPS classes. Extensive development of extraction techniques has allowed for reduction of matrix effects while targeting low limits of detection in smaller and smaller sample volumes. Optimization of chromatography has been key for separating isomers while still maintaining short runtimes. Advanced mass spectrometric acquisition methods have been designed for screening, identifying, and quantifying these NPS in forensic specimens. We discuss analytical techniques for quantification of synthetic cathinones and screening of fentanyl analogs by LC-QTOF. Additionally, we discuss methods for quantification of synthetic opioids by LC-QQQ. Differences in approaches between the two types of technologies are compared and contrasted.

The fully optimized and validated techniques have been applied to analyze forensic toxicology specimens, study drug stability in biological fluids, investigate drug metabolism pathways, understand postmortem redistribution, and identify novel psychoactive substances. High-resolution mass spectra have been particularly key in developing libraries, characterizing unique biomarkers and metabolites, and identifying novel psychoactive substances from their closely related isomers and analogs.

Understanding pharmacology of emerging compounds is highly reliant upon advanced analytical techniques that allow us to characterize their activity and stability in biological samples or identify metabolites in in vitro assays so that we can better interpret toxicological findings in routine specimens.

Detailed Learning Objectives:

- Understand differences of quantitative assays by LC-QQQ and LC-QTOF.
- Identify key steps of method development that allow for sensitive methodologies.
- Appreciate different approaches to mass spectral data acquisition in LCMSMS.

Dr. Kerrigan, Presentation PDF: https://mp634935.cdn.mediaplatform.com/634935/wc/mp/predeploy/67/_67a8038d-022b-a67b-e7e1-6c3e1bce1882_/Forensic-toxicology-symposium-day2-speaker3-pp-agilent.pdf

Dr. Kerrigan, Slides and Transcript: https://mp634935.cdn.mediaplatform.com/634935/wc/mp/predeploy/ca/_ca1c2834-e164-8da2-663a-8363dee0e731_/Forensic-toxicology-symposium-day2-speaker3-pp-agilent.pptx

Dr. Swortwood, Presentation PDF: https://mp634935.cdn.mediaplatform.com/634935/wc/mp/predeploy/28/_2882b180-2681-0426-35b0-f18929f77a18_/Forensic-toxicology-symposium-day2-speaker2-pp-agilent.pdf

Dr. Swortwood, Slides and Transcript: https://mp634935.cdn.mediaplatform.com/634935/wc/mp/predeploy/a4/_a4f8a3ed-ff7b-b656-3fd5-311419bdbb44_/Forensic-toxicology-symposium-day2-speaker2-pp-agilent.pptx

Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

1. Coping with Requirements in Forensic Toxicology: Combination of Routine Laboratory and Forensic Science
   Prof. Stefan W. Toennes, PhD
2. LC/MS/MS Approaches for Identifying Emerging NPS
   Sarah Kerrigan, PhD, and Madeleine Swortwood, PhD

Day 3–Thursday

Posters

Resources

Call for Abstracts

PRESENTATIONS

Archival Registration: https://forensicrti.org/course/virtual-online-symposium-current-trends-in-forensic-toxicology-agilent/

Sarah Kerrigan, PhD, Professor and Chair, Department of Forensic Science, Sam Houston State University, Huntsville, Texas

Dr. Sarah Kerrigan is Chair of the Department of Forensic Science at Sam Houston State University. She has more than 20 years' experience as a practitioner and researcher in forensic toxicology. She is a former state laboratory director and quality assurance manager.

Sarah Kerrigan, PhD

Madeleine Swortwood, PhD, Assistant Professor, Department of Forensic Science, Sam Houston State University, Huntsville, Texas

Dr. Madeleine Swortwood has more than 8 years' research experience with NPS by LC/MS/MS. She was a former post-doctoral fellow at the National Institute on Drug Abuse (NIDA) and has more than 19 peer-reviewed publications for analytical methodologies and alternative matrices.

Madeleine Swortwood, PhD

PRESENTATIONS

Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

Day 3–Thursday

1. In Vitro Biotransformation of New Psychoactive Substances
   Prof. Alexander van Nuijs, PhD
2. Screening and Confirmation Strategies in Postmortem Toxicology
   Robert Kronstrand, PhD

Posters

Resources

Call for Abstracts

Day 3

1. In Vitro Biotransformation of New Psychoactive Substance

VIEW RECORDING

ANNOTATED SLIDES

Prof. Alexander van Nuijs, PhD, Toxicological Centre, University of Antwerp, Belgium

Abstract: The use of new psychoactive substances (NPS) may pose a public health threat because there is little to no scientific evidence of their pharmacokinetics, recommended dose, effects, or safety. Furthermore, NPS can be easily acquired through the internet and smart shops, where NPS are sold under various product labels—often with misleading information. From a forensic point of view, NPS are very challenging as there is little information available regarding the metabolic fate of these new substances. The detection in various biological fluids is therefore difficult and possible false positives or false negatives may occur. Characterization of the biotransformation of NPS is important in order to identify suitable biomarkers to be used in forensic screening.

This presentation will present in vitro techniques and workflows to elucidate the Phase-I and Phase-II biotransformation of NPS. Experimental setups for incubations with pooled human liver microsomes and cytosol to generate Phase I and Phase II biotransformations will be shown and discussed, including positive and negative controls. Resulting extracts from the incubations are analyzed with liquid chromatography coupled to quadrupole time-of-flight mass spectrometry (LC-QTOF-MS). Data analysis for identifying biotransformation products with three different data-analysis workflows will be discussed. A suspect screening workflow was developed using an in-house prepared database built from literature data and in silico biotransformation predictions with the Meteor Nexus software (Lhasa Limited). Furthermore, two non-target screening methods were optimized and applied: (i) using the Agilent MassHunter Qualitative software and (ii) using the open-source software MZmine 2.29 for mass spectrometry data processing. The obtained m/z features were further processed and visualized using R software.

Examples of the techniques and workflows will be given for several classes of NPS such as benzodiazepines (cloniprazepam) and synthetic cannabinoids (5-Cl-THJ-018). For 5-Cl-THJ-018, the results obtained through the in vitro experiments are compared with in vivo results (urine from a 5-Cl-THJ-018 user) to confirm the suitability of the in vitro setup

Detailed Learning Objectives:

- Develop an in vitro experimental design for investigation of biotransformation of compounds.
- Review examples and comparison of multiple data analysis workflows (both suspect- and non-target screening).
- Elucidate the metabolic pathway (Phase-I and Phase-II reactions) of several NPS.

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Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

Day 3–Thursday

1. In Vitro Biotransformation of New Psychoactive Substances
   Prof. Alexander van Nuijs, PhD
2. Screening and Confirmation Strategies in Postmortem Toxicology
   Robert Kronstrand, PhD

Posters

Resources

Call for Abstracts

PRESENTATIONS

Prof. Alexander van Nuijs, PhD, Toxicological Centre, University of Antwerp, Belgium

Dr. Alexander van Nuijs is professor in the Department of Pharmaceutical Sciences at the University of Antwerp. His main research area is forensic and analytical toxicology. He has expertise in the analysis of a wide range of analytes (e.g., illicit drugs, pharmaceuticals, toxicants) in different matrices (e.g., blood, urine, hair, nails, wastewater). One of his main research topics is the investigation of the in vitro biotransformation of new psychoactive substances with the aim to elucidate metabolic pathways.

Prof. Alexander van Nuijs, PhD

Foreword

Presentations

Day 1–Tuesday

Day 2–Wednesday

Day 3–Thursday

1. In Vitro Biotransformation of New Psychoactive Substances
   Prof. Alexander van Nuijs, PhD
2. Screening and Confirmation Strategies in Postmortem Toxicology
   Robert Kronstrand, PhD

Posters

Resources

Call for Abstracts

PRESENTATIONS

2. Screening and Confirmation Strategies in Postmortem Toxicology

VIEW RECORDING

ANNOTATED SLIDES

Robert Kronstrand, PhD, Toxicologist, National Board of Forensic Medicine, Sweden

Abstract: Systematic toxicological analysis is the pillar of postmortem forensic toxicology. It includes the detection, identification, and quantitation of a range of substances including gases, metals, anions, volatiles, pesticides, medications, and drugs of abuse. However, most forensic toxicology laboratories use a case-based progression in their analytical strategy that includes the communication with police and the medical examiner. The reason for this, of course, is cost effectiveness. On the other hand, a good general rule is to have a tier-one panel of screening analyses that is always performed and that can detect and exclude a broad range of relevant substances. Confirmatory analyses always include identification and most of the times also quantitation to enable a correct interpretation.

The aim of this lecture is to describe the possibilities that different screening approaches offer and problematize different workflows for screening and confirmation analyses in a forensic laboratory with focus on postmortem toxicology. The lecture mainly covers analytical strategies for medications and drugs of abuse, including new psychoactive substances; the lecture is built around the experience from working more than 25 years in a large-scale forensic laboratory that handles thousands of autopsy cases on a yearly basis.

Detailed Learning Objectives:

- Recognize the pros and cons of different techniques and methodologies.
- Evaluate and select appropriate methodology for the analysis of drugs in postmortem cases.
- Design strategies for successful screening and confirmation.

Presentation PDF: https://mp634935.cdn.mediaplatform.com/634935/wc/mp/predeploy/a7/_a7a49f16-c1c4-23cf-7970-27845e6f71db_/Forensic-toxicology-symposium-day3-speaker2-pp-agilent.pdf

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Archival Registration: https://forensicrti.org/course/virtual-online-symposium-current-trends-in-forensic-toxicology-agilent/

Robert Kronstrand, PhD, Toxicologist, National Board of Forensic Medicine, Sweden

Dr. Robert Kronstrand is the Research Strategist for the National Board of Forensic Medicine (NBFM) in Sweden. He joined the NBFM's Department of Forensic Toxicology in 1990 and later received his PhD in human toxicology in 2001. He has more than 25 years of experience in studying postmortem toxicology, driving under the influence of drugs (DUID), and drug-facilitated sexual assault (DFSA); additionally, he has published more than 70 papers about forensic and analytical toxicology. He also holds a position as professor in forensic toxicology at the Faculty of Medicine and Health Sciences, Linköping University.

Robert Kronstrand, PhD

Foreword

Presentations

Posters

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS
2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System
3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS
4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC
5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS
6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ
7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry
8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis
9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS
10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ
11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

Resources

Call for Abstracts

POSTERS

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS

VIEW POSTER

Joan Stevens and Limian Zhao, Agilent Technologies, Inc.

Efficient extraction, cleanup, and analysis of complex biological samples are extremely beneficial to the forensic laboratory. Phospholipids (PPLs) have been identified as a major cause of matrix effects in the LC-MS/MS analysis of tetrahydrocannabinol (THC) and its metabolites in whole blood. This Application Note describes the extraction and LC-MS/MS analysis of Δ9-THC (THC) and its major metabolites, 11-hydroxy-Δ9-THC (THC-OH) and 11-nor-9-carboxy-Δ9-THC (THC-COOH) from whole blood using in-well PPT followed by PPL removal using Agilent Captiva EMR—Lipid in a pass-through 1 mL cartridge. Captiva EMR—Lipid produced cleaner eluents with removal of over 97 % of the unwanted PPLs from whole blood matrix, and over 92 % recoveries for target analytes. Analysis of THC, THC-OH, and THC-COOH at 1 ng/mL yielded ideal peak shapes with good signal-to-noise (S/N). Response from 0.5 to 100 ng/mL was linear, with an R2 >0.99. Limits of quantitation of 1.0 ng/g or lower were obtained, with RSD <11.5 %. Results were consistent over three days of experiments.

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2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System

VIEW POSTER

Kirk E. Lokits, Raymond J. Kuk, Michelle Clarke, Graham Robinett & Eric Pavlich

Analysis of ignitable liquids (ILs) and ignitable liquid residues (ILRs) by the fire debris analyst, has routinely utilized capillary chromatography with mass selective detectors (MSD). The total ion chromatogram (TIC) pattern of peaks representing components found in various ILs and can be compared to patterns from known IL references. The MSD provides additional selectivity and permits structural identification of the specific compounds found in (IL) and (ILRs). The purpose of this research is to demonstrate that several recent advances in gas chromatography, found in the Agilent Technologies Intuvo 9000 GC, can be successfully incorporated into the current proven methods of fire debris analysis. This work seeks to show that this can be done with minimal disruption to the established practices of data acquisition and data analysis while demonstrating the improvements that can be derived from recent developments in GC technology. Method translation software was used in this study to convert an existing fire debris GC method with a runtime of 38 minutes to a fast GC method with a runtime of 19 minutes. The fast GC method is achieved without changing the peak elution or negatively affecting peak resolution.

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Foreword

Presentations

Posters

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS
2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System
3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS
4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC
5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS
6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ
7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry
8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis
9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS
10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ
11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

Resources

Call for Abstracts

POSTERS

3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS

VIEW POSTER

Limian Zhao

Determination of abuse drugs (DoA) in whole blood has been considered as the first choice for the quantitative analysis of DoAs in clinical research labs. Therefore, a solid quantitative analytical method is critical to achieve accurate and reliable results. Biological sample matrix like whole blood is very complex, containing endogenous and exogenous substances. It is also quite viscous and difficult to handle. Therefore, appropriate sample preparation is critical to extract target analytes, clean unwanted matrix interferences, and also simplify the sample operation. In addition, the 96-well plated based sample preparation has been widely used for high-throughput bioanalysis for quantitative determination of target analytes in biological matrices, due to its batch process and automatable operations, and also limited sample volume used for biological sample analysis.

Captiva EMR-Lipid plate provides pass-through matrix cleanup to remove major lipid substances from sample matrix without unwanted analyte loss. By selectively interacting with the long aliphatic chain of the lipid compounds, the EMR-Lipid cleanup provides efficient phospholipids and other classes of lipids from biological fluids after protein precipitation (PPT). The highly selective interaction mechanism also assures minimal retention of target analytes during cleanup. In addition, the in-well protein precipitation reduces the sample transfer and allows automatic operation. All of the features above make Captiva EMR-Lipid cleanup an excellent option to prepare samples for DoA analysis in whole blood in clinical research studies.

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4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC

VIEW POSTER

Kevin McCann, Andre Szczesniewski & Pete Stone

Liquid chromatography triple quadrupole mass spectrometry (LC/MS/MS) provides excellent testing specificity and accuracy with rapid analysis times. However, many forensic labs are interested in improving sample throughput to better utilize their testing instrumentation. While analysis times can be shortened through appropriate LC method choices, a user is often only interested in a portion of the total data collected by an LC/MS system. Typically, there is time during each chromatographic separation where no compounds of interest are being analyzed by the mass spectrometer, leaving the instrument under-utilized for a large period of time.

This work demonstrates the ability to increase mass spectrometer productivity for the analysis of Δ^9-tetrahydrocannabinol (THC) through the automated use of a dual channel high performance liquid chromatography (HPLC) system. A newly developed software interface intelligently determines the timing of all HPLC components and coordinating the analytical utilization of the mass spectrometer.

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Foreword

Presentations

Posters

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS
2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System
3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS
4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC
5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS
6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ
7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry
8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis
9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS
10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ
11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

Resources

Call for Abstracts

POSTERS

5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS

VIEW POSTER

Mohamed Youssef, Nikunj Parikh, Vaughn Miller & William

New high throughput methods are desired to overcome the increasing number of samples requiring analysis in clinical research and forensic toxicology laboratories. Ultrafast SPE/MS/MS systems are capable of analyzing many analytes in biological matrices at a rate of 11-15 seconds per sample. In the present study, we evaluated the capabilities of the Agilent RapidFire High-throughput Mass Spectrometry, an ultrafast SPE/MS/MS system, to quantitatively measure multiple drug panels in human urine; methadone (and its metabolite), and buprenorphine (and its metabolite). The results were then compared to traditional LC/MS/MS analysis.

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6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ

VIEW POSTER

Julian Delamata, Xiaomi Xu, Tarun Anumol, Joan Stevens & Limian Zhao

Per/Polyfluoroalkyl substances (PFASs) are widely used in manufacture and industry because of their desirable properties. They find uses as surfactants, fire-retardants, non-stick cookware and other applications. Their unique properties also make them persistent with long half-lives. Studies have shown that the longer (C-chain>7) PFAS can be bio-accumulative. PFASs are ubiquitous and known to be found in blood and serum. A method was developed for the detection of PFASs in plasma using a novel lipid removing sorbent Captiva EMR-Lipid in a flow through format and Agilent 6495 Triple Quadrupole LC/MS.

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Foreword

Presentations

Posters

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS
2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System
3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS
4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC
5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS
6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ
7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry
8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis
9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS
10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ
11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

Resources

Call for Abstracts

POSTERS

7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry

VIEW POSTER

Martin Josefsson, Bernhard Wuest, Markus Roman

In recent years accurate mass TOF and Q-TOF mass spectrometers have become more standard in forensic toxicology laboratories. The need to analyze unknown drugs and their metabolites requires sophisticated software tools to handle accurate mass data. We developed a novel algorithm which enables unprecedented accuracy in identification of drugs and their metabolites. The identification of isomeric compounds without the need of a standard is particularly important as many metabolite standards are not commercially available. The use of a co-elution score makes is possible to find fragments without a priori knowledge of the fragmentation.

In this study, post-mortem blood samples were analyzed to evaluate the ability of the All Ions MS/MS algorithm to correctly identify isobars and isomers. By combining MS and MS/MS experiments with All Ions MS/MS, users gain increased analytical speed and accuracy, significantly improved identification of compounds of interest, and increased productivity in forensic toxicology laboratories. Laboratories that analyze panels of drugs can import All Ions MS/MS results directly into their MassHunter Quantitative Analysis software for more productive identification and quantitation in a single software package.

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8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis

VIEW POSTER

Limian Zhao & Derick Lucas

Lipids, especially phospholipids (PPLs), in biological matrices can significantly impact bioanalysis quality by LC/MS/MS. The unremoved phospholipids and matrix interferences can cause significant ion suppression, resulting in lower detection limits and poor method reliability, resulting in lower productivity and eventual financial losses.

Agilent Enhanced Matrix Removal–Lipid (EMR–Lipid) is a series of new products utilizing a novel sorbent material that selectively removes major lipid classes from sample matrix without unwanted analyte loss. The lipid removal mechanism is a combination of size exclusion and hydrophobic interaction between the long aliphatic chain of the lipid substances and the EMR–Lipid sorbent. The selective interaction mechanism allows efficient removal of phospholipids and other classes of lipids from biological fluids after PPT.

Captiva EMR–Lipid is a new pass-through cleanup product implemented in a convenient SPE cartridge or 96-well plate format. The use of Captiva EMR–Lipid products provides > 99 % phospholipids removal and clogging-free, easy elution for in-situ protein precipitation. The 96-well Captiva EMR–Lipid plate was evaluated for the quantitative determination of representative drug compounds in human serum by LC/MS/MS. The results demonstrated that the established protocol using in-situ PPT followed by Captiva EMR–Lipid cleanup provides significant improvements for the reliable quantitative determination of drug compounds in biological matrices.

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Foreword

Presentations

Posters

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS
2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System
3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS
4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC
5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS
6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ
7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry
8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis
9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS
10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ
11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

Resources

Call for Abstracts

POSTERS

9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS

VIEW POSTER

Peter JW Stone

Opiates and their metabolites can be challenging to analyze using LC/MS due to a relatively large number of their analytes having the identical empirical mass and subsequent similar fragmentation patterns in MS/MS. The need for good chromatographic separation is therefore paramount as is the need to reduce complicated sample preparation techniques.

Opiate glucuronides pose the greater separation challenge in reverse phase chromatography due to their highly polar nature and are, therefore, routinely hydrolyzed during sample preparation, a process that removes any sugar group returning the metabolite to its original parent form.

Acid and enzyme hydrolysis stages of sample preparation can be relatively lengthy processes so this research project set out to investigate the scientific feasibility of separating and measuring common opiates, metabolites and glucuronide metabolites directly and in one quick analytical method.

A five minute LC/MS MRM method was developed which chromatographically separated each of the isobaric analytes outlined in table 1. Results were obtained for five batches of spiked urine samples over the concentration range of 0.5-1000ng/ml. Precision data obtained and calibration accuracies will be reported for each analyte.

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10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ

VIEW POSTER

Peter JW Stone

During this research study, a sensitive, robust and relatively fast targeted analytical method was developed for the quantitation of 12x synthetic fentanyl opioids, 4-ANPP the synthetic precursor molecule and a similar powerful opioid-like synthetic known as W-18. Simple sample preparation routines were employed to make samples ready for analysis using an Ultivo triple quadrupole mass spectrometer LC/MS (LC/TQ) from both human serum and urine matrices.

Several separate batches were prepared and analyzed for the purpose of obtaining statistically valid analytical performance results in this research study and the resultant lower limits of quantitation, chromatographic precision, calibration linearity, range and accuracy for each synthetic opioid will be presented herein. A comparison of the analytical performance of each analyte for both urine and serum matrices will also be outlined.

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Foreword

Presentations

Posters

1. Efficient Quantitative Analysis of THC and Its Metabolites in Whole Blood Using Agilent Captiva EMR—Lipid and LC-MS/MS
2. Accelerating the Analysis of Ignitable Liquids and Ignitable Liquid Residues on the Agilent Technologies GCMS 5977B/Intuvo 9000 System
3. Multi-residue Analysis of Abuse Drugs in Whole Blood Using In-well Protein Precipitation Followed with Captiva EMR-Lipid Cleanup by LC/MS/MS
4. Increased Throughput for the Analysis of Δ9-tetrahydrocannabinol (Δ9-THC) in Oral Fluids Using Triple Quadrupole Mass Spectrometry Coupled to Automated Dual-Channel HPLC
5. Ultrafast, Quantitative Analysis of Buprenorphine, Methadone, and Their Metabolites in Human Urine Using Online SPE/MS/MS
6. Analysis of Per/Polyfluoroalkyl Substances (PFASs) in Biological Fluid Using a Novel Lipid Removing Sorbent and LC/TQ
7. New Algorithms Using All Ions MS/MS for the Identification of Isobaric Drugs in Blood Samples Using LC/MS/MS High Resolution Mass Spectrometry
8. Enhanced Lipids Removal from Biological Matrices to Prepare Samples for LC/MS/MS Analysis
9. The Separation and Analysis of Opiates and Their Glucuronide Metabolites in Urine Matrix Negating the Need for Hydrolysis During Sample Preparation Using Tandem LCMS/MS
10. The Detection and Analytical Confirmation of Synthetic Fentanyl Analogues in Human Urine and Serum Using an Ultivo LC/TQ
11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

Resources

Call for Abstracts

POSTERS

11. Analysis of Explosive Materials and Explosive Residue on Contaminated Matrices Utilizing the Agilent Technologies GCMS 5977A/9000 Intuvo System Using Hydrogen as a Carrier Gas

VIEW POSTER

Kirk E. Lokits, Graham Robinett & Eric Pavlich

Analysis of explosives and explosive residues, has routinely utilized gas chromatography with mass selective detectors (MSD). The MSD provides sensitivity, selectivity, and permits structural identification of the specific compounds found in explosives and residue matrices. The purpose of this research is to demonstrate that several recent advances in gas chromatography, found in the Agilent Technologies 9000 Intuvo GC, can be successfully incorporated into current proven methods of explosive analysis. The advancements in GC design facilitates the Intuvo to be a viable remedy for a field mobile GCMS solution. This work seeks to illustrate this with minimal disruption to the established practices of data acquisition and analysis while demonstrating the improvements that can be derived from recent developments in GC technology. In addition, due to the common weight and space limitations for a mobile laboratory, H2 was utilized as the carrier gas, thus eliminating the need for compressed gas cylinders since a reliable source of H2 can easily be produced using a variety of hydrogen generators on the market. This study utilizes an existing conventional explosives GCMS method, that incorporates H2 as its carrier gas and depicts good peak shape and sensitivity, without excessive peak tailing or negatively affecting peak resolution. However, using H2 carrier can cause reactions during fragmentation (especially nitrogen and oxygen containing compounds) resulting in non-standard EI spectra and spectral differences when compared to He carrier gas applications. In an attempt to mediate spectral differences, an in-house library was produced under H2 carrier gas conditions and used for comparative purposes.

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Foreword

Presentations

Posters

Resources

Peer-Reviewed Papers

Webinars

Drug Library Resources

Video Resources

Agilent Resource Materials

Call for Abstracts

RESOURCES

Peer-Reviewed Papers

Identification of Suvorexant in Urine Using Liquid Chromatography-Quadrupole/Time-of-Flight Mass Spectrometry (LC-Q/TOF-MS)

Sydney Sullinger, Kelsie Bryand, Sarah Kerrigan

Journal of Analytical Toxicology, Volume 41, Issue 3, 1 April 2017, Pages 224–229

https://academic.oup.com/jat/article/41/3/224/2758297?searchresult=1

Developing a UHPLC–QTOF-MS and Automated Library Search Method for Screening Drugs and Toxic Compounds in Postmortem Specimens

Hsiu-Chuan Liu, Chu-An Yang, Ray H. Liu, Dong-Liang Lin

Journal of Analytical Toxicology, Volume 41, Issue 5, 1 June 2017, Pages 421–430

https://academic.oup.com/jat/article/41/5/421/3084597?searchresult=1

Simultaneous Quantitation of Methamphetamine, Ketamine, Opiates and their Metabolites in Urine by SPE and LC–MS-MS

Chu-An Yang, Hsiu-Chuan Liu, Dong-Liang Lin, Ray H Liu, You-Zung Hsieh ...

Journal of Analytical Toxicology, Volume 41, Issue 8, 1 October 2017, Pages 679–687

https://academic.oup.com/jat/article/41/8/679/3978801?searchresult=1

Confirmation of Carfentanil, U-47700 and Other Synthetic Opioids in a Human Performance Case by LC–MS-MS

Joshua Seither, Lisa Reidy

Journal of Analytical Toxicology, Volume 41, Issue 6, 1 July 2017, Pages 493–497

https://academic.oup.com/jat/article/41/6/493/3926148?searchresult=1

Analysis of Novel Synthetic Opioids U-47700, U-50488 and Furanyl Fentanyl by LC–MS/MS in Postmortem Casework

Amanda L. A. Mohr, Melissa Friscia, Donna Papsun, Sherri L. Kacinko, David Buzby ...

Journal of Analytical Toxicology, Volume 40, Issue 9, 16 November 2016, Pages 709–717

https://academic.oup.com/jat/article/40/9/709/2527448?searchresult=1

Validation of LC–TOF-MS Screening for Drugs, Metabolites, and Collateral Compounds in Forensic Toxicology Specimens

Fessessework Guale, Shahriar Shahreza, Jeffrey P. Walterscheid, Hsin-Hung Chen, Crystal Arndt, Anna T. Kelly; Ashraf Mozayani

Journal of Analytical Toxicology, Volume 37, Issue 1, 1 January 2013, Pages 17–24

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Foreword
Presentations
Posters
Resources
Peer-Reviewed Papers
Webinars
Drug Library Resources
Video Resources
Agilent Resource Materials
Call for Abstracts

RESOURCES

Webinars

Method Validation for Quantitation and Confirmation of Amphetamines, Phentermine, and Designer Stimulants by LC/MS/MS

Dr. Rebecca L. Wagner, Research Analyst for the Virginia Department of Forensic Science

https://rticqpub1.connectsolutions.com/content/connect/c1/7/en/events/event/shared/1206901504/event_landing.html?sco-id=1206904914&_charset_=utf-8

Fast Quantitative Analysis of THC and Its Metabolites in Biological Samples Using Captiva EMR-Lipid and LC/MSMS

Christophe Deckers, MSc, Sample Prep Application Scientist, Agilent Technologies, Inc.

https://agilenteseminar.webex.com/...

New Synthetics and New Forensic Innovations. Synthetic Fentanyl Analogues and the New Agilent Ultivo Tandem MS

Julie Cichelli, Application Engineer, Agilent Technologies, Inc.

https://agilenteseminar.webex.com/...

Exploiting the Power of LCTOF Data Mining

Barry Logan, PhD, F-ABFT, Chief Scientist, NMS Labs

https://rti.connectsolutions.com/p53ay0dh980/?launcher=false&fcsContent=true&pbMode=normal

Power of High Res Mass Spectrometry to Detect Fentanyl Analogues

Curt E. Harper, PhD, F-ABFT, and Jason Hudson, PhD, F-ABFT, of the Alabama Dept. of Forensic Sciences

www.agilent.com/en/video/analyze-fentanyl-analogues

Robotic Extraction and LC/MS/MS Forensic Analysis of Insulin Analogs

Kevin Legg, PhD, Research Scientist, The Center for Forensic Science Research & Education, Willow Grove, PA

https://www.agilent.com/en/training-events/eseminars/robotic-extraction-forensic-analysis

DART-TOF MS Screening of Fentanyl

Curt E. Harper, PhD, F-ABFT, Toxicology Discipline Chief, and Erin M. Shonsey, PhD, Director of Research, Alabama Dept. of Forensic Sciences

https://www.agilent.com/en/training-events/eseminars/dart-tof-ms-screening-of-fentanyl

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Foreword
Presentations
Posters
Resources
Peer-Reviewed Papers
Webinars
Drug Library Resources
Video Resources
Agilent Resource Materials
Call for Abstracts

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Video Resources

Learn from your colleagues about their experiences with LC/TOF and LC/Q-TOF

Increasing the Scope of Analytical Detection with LC/TOF/Q-TOF at NMS Labs

Barry Logan, PhD, NMS Labs

https://www.agilent.com/en-us/solutions/forensics/increasing-the-scope-of-analytical-detection

Detecting a Broad Range of Drugs at the Alberta Medical Examiner's Office

Graham Jones, PhD, Alberta Medical Examiners Office

https://www.agilent.com/en-us/solutions/forensics/detecting-a-broad-range-of-drugs

Identifying Novel Psychoactive Substances (NPS) at the University of Antwerp

Adrian Covaci, Professor of Environmental & Forensic Toxicology, University of Antwerp, Belgium

https://www.agilent.com/en/video/identify-psychoactive-substances

Agilent Resource Materials

Agilent LC/MS Instruments
https://www.agilent.com/en/products/mass-spectrometry/lc-ms-instruments

Agilent Analyzers, Databases, and Libraries
https://www.agilent.com/en/products/mass-spectrometry/analyzers-databases-libraries#1

Agilent Technology Refresh Program for Forensics Labs
https://www.agilent.com/cs/library/brochures/5991-9012EN_Forensic_refreshprogram_brochure.pdf

Ultivo Triple Quadrupole Mass Spectrometer Brochure
https://www.agilent.com/cs/library/brochures/5991-8146EN.pdf

QQQ LC/MS Forensic Toxicology MRM Database and Application Kit Flyer
https://www.agilent.com/cs/library/brochures/5990-5640EN.pdf

Agilent 6400 Series Triple Quadrupole LC/MS Systems
https://www.agilent.com/cs/library/brochures/5990-9758en_hi.pdf

Raise Your Analysis to a New Level: Agilent 6530 Q-TOF LC/MS System
https://www.agilent.com/cs/library/brochures/5991-9063EN_6530_brochure.pdf

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Posters
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Agilent Technologies, in partnership with ForensicRTI, invites abstract submissions for poster presentations that will be held at the second annual Online Virtual Forensic Symposium in May 2019. The poster session will be available to attendees throughout the week. There is no requirement for the authors to be available while the posters are being viewed. Submitted posters will be made available along with the recorded oral presentations for archival/post-event viewing. Posters presented at other meetings i.e. TIAFT, SOFT, etc will be considered without the need for updating or modifying content.

The Online Virtual Forensic Symposium provides virtual attendees with ready access to some of today's leading researchers and practitioners without ever needing to leave the laboratory; the event also provides the opportunity for virtual audience members to remain current on critical issues facing today's forensic toxicologists.

Proposal submission closes on **Friday, March 1, 2019**.

Proposals should include the following:

1. Title of abstract: (no more than 80 characters)
2. Presentation abstract: (500–1,000 words to describe the scope, objectives, and narrative of the presentation; the presentation abstract will be used for the selection process.)
3. Upload of the abstract

For questions regarding this event, please contact forensics@rti.org.

Link for submissions: https://forensicrti.org/agilent-abstractsubmissions/

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