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>> WELCOME MESSAGE

Scientific Program Chairs:

Welcome to the 2024 Current Trends in Seized Drug Analysis Symposium. We look forward to a week of exciting interactions with scientists and law enforcement agencies worldwide who will show how drug analysis methods and data can be used in the fight against drugs and organized crime.

Traditionally, drug analysis has been a reactionary field, where analysis strategies are developed after the arrival of new illicit substances on the market or detection technologies that have evolved after new smuggling methods are unearthed. This year's symposium will focus upon efforts to hinder the flow of illicit substances onto the market through finding the sources, tracking the distribution networks and using analysis data to probe and understand the drug market (both on the street and on the Internet). In this light, we have chosen the theme "Ahead of the Game" this year. The presentations will take us from Clandestine Labs (Day I), Chemical Profiling (Day 2), Cannabis: Life After Legislation (Day 3), Forensic Intelligence (Day 4) to Emerging Technologies (Day 5). We will learn how we can smartly use of science and technology to minimize the flow of narcotics onto the market.

There is a daily discussion panel at 11:30 EST. You are encouraged to actively participate by asking questions in the symposium's chat function and sharing your expertise with the community. Each day is also complemented by a workshop, vendor presentations, and posters. We are grateful for the dedication of our presenters, many of which are joining us from different continents and time zones. We hope this event will be informative, enjoyable, and inspiring.



Simon Dunne - Chair



Maggie Tam - Co-Chair

>> SYMPOSIUM 2024



Simon Dunne Scientific Program Chair

Simon Dunne is a forensic specialist working at the National Forensic Centre within the Swedish Police Authority. As the research coordinator for the Drug Analysis section Simon's work focusses upon methods for the detection and identification of new psychoactive substances, semi-automatic methods for chemical profiling of narcotics, the use of hyperspectral NIR imaging for determination of the identity and homogeneity of narcotics seizures, together with rapid screening using non-destructive spectroscopic techniques combined with tandem applications of unsupervised/supervised chemometric methods.

Maggie Tam, PhD CChem Scientific Program Co-Chair

Senior Research Scientist, Canada Border Services Agency

Maggie Tam is a senior research scientist at the Canada Border Services Agency. As a subject matter expert in drugs and explosives detection and identification, she evaluates field equipment and conducts applied research for border security applications. She is a co-instructor for the Short Course on Ion Mobility Spectrometry at the International Conference on Ion Mobility Spectrometry. She is Past President of the International Society for Ion Mobility Spectrometry (ISIMS) and Trustee for the Scientific Workshops. She champions for equity, diversity and inclusion through her involvement with the Leadership Development Committee of Females in Mass Spectrometry (FeMS).





Dr. Tom Gluodenis
Symposium Organizer
Associate Professor, Lincoln University, PA

linkedin.com/in/tgluodenis

Dr. Tom Gluodenis earned a PMFS from Florida International University, an EMBA from St. Joseph University in Philadelphia and his MSc. and Ph.D.in analytical chemistry from the University of Massachusetts, Amherst. He spent 23 years with Hewlett-Packard/Agilent Technologies and retired in 2019 from his role as Global Marketing Manager for Forensics & Forensic Toxicology. In that role, Dr. Gluodenis was an expert resource on forensic trends, regulations, technologies, and testing protocols while coordinating countless partnerships & collaborations with practitioners and researchers around the globe. Currently, Dr. Gluodenis is an Associate Professor at Lincoln University in Pennsylvania and founder of the highly acclaimed online symposium series, Current Trends in Forensics & Forensic Toxicology which has provided continuing education to over 6000 students, educators, and practitioners in over 80 counties. He is a past member of the Seized Drug subcommittee of the NIST OSAC and the Toxicology section of the American Standards Board. He is a member of several national and international forensic organizations including the Society of Forensic Toxicologists where he serves on the Diversity Committee, the American Academy of Forensic Sciences, the International Association of Forensic Toxicologists where he serves on the Continuing Education Committee, and the Forensic & Clinical Toxicology Association of Australasia.





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Clandestine Labs

8:45am EST - 9:00am EST | 1:45pm GMT - 2:00pm GMT

Welcome & Introduction

Program Chairs Simon Dunne & Maggie Tam

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Adapting to Dynamic Illicit Drug Lab Operations in the United States

Dean Kirby, Senior Research Chemist, Drug Enforcement Administration, Special Testing and Research Laboratory, Dulles, Virginia USA

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

Visualizing Contamination from Drugs and Homemade Explosives

Matthew Staymates, National Institute of Standards and Technology

10:00am EST - 10:15am EST | 3:00pm GMT - 3:15pm GMT Morning Break

10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

Clandestine Production Labs in the Netherlands, a Daily Challenge

Dr. Sander Oldenhof, Drug Expert at the Netherlands Forensic Institute

10:45am EST - 11:00pm EST | 3:45pm GMT - 4:00pm GMT

What's New on the Designer Drug Scene: Synthetic Cannabinoids, Precursors, and More (sponsored)

Holly Pierzynski, MS, Manager of Forensic Novel Psychoactive Substance Research, Cayman Chemical

II:00am EST - II:30pm EST | 4:00pm GMT - 4:30pm GMT

Clandestine Laboratory Trends and Challenges in Western Canada

Adrienne Law, Clandestine Laboratory Specialist, Drug Analysis Services Laboratory, Health Canada

II:30am EST - I2:00pm EST | 4:30pm GMT - 5:00pm GMT

Panel Discussion with All Presenters

1:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

Delving into the World of Lyseramides: The Past, Present, and Future (Cayman Chemical Sponsored Workshop)



Chemical Profiling

8:45am EST - 9:00am EST | I:45pm GMT - 2:00pm GMT

Welcome & Introduction

Program Chairs Simon Dunne & Maggie Tam

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Australian Illicit Drug Trends and Profiling Insights

Ms Erin Ellis and Miss Kirra King – Australian Federal Police Forensic Drug Intelligence Analysts

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

A Forensic Perspective to the Chemical Profiling of Illicit Drugs

Sami Huhtala, National Bureau of Investigation, Finland

10:00am EST - 10:15am EST | 3:00pm GMT - 3:15pm GMT

Morning Break

10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

DEA's Chemical Profiling - Drug Intelligence from the Lab

Joe Bozenko, Senior Research Chemist, DEA Special Testing & Research Laboratory

10:45am EST - 11:00pm EST | 3:45pm GMT - 4:00pm GMT

Spectral libraries for detection & identification of NPS (sponsored)

Tim Stratton, Manager Library Technologies, Thermo Fisher Scientific

II:00am EST - II:30pm EST | 4:00pm GMT - 4:30pm GMT

Profiling in Real Time: Combining Chemical Correctness with Big Data Analysis

Simon Dunne, National Forensic Center (NFC), Swedish Police Authority, Sweden

II:30am EST - I2:00pm EST | 4:30pm GMT - 5:00pm GMT

Panel Discussion with All Presenters

1:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

Advances in Mass Spectrometry for High Throughput Drug Testing (Thermo Fisher Scientific Sponsored Workshop)



Wednesday - January 24th, 2024

Cannabis: Life After Legalization

8:45am EST - 9:00am EST | 1:45pm GMT - 2:00pm GMT

Welcome & Introduction

Program Chairs Simon Dunne & Maggie Tam

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

The Impact of Cannabis Legalization on Poisonings

Dr Rose Cairns, Senior Lecturer in Pharmacy, The University of Sydney; and Director of Research, New South Wales Poisons Information Centre, Sydney, Australia

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

The EU Market for Cannabis: Increasing Complexity Poses Higher Risks to Users' Health and Challenges to Policymakers

Laurent Laniel, principal scientific analyst, markets, crime and supply reduction, EMCDDA

10:00am EST - 10:15am EST | 3:00pm GMT - 3:15pm GMT

Morning Break

10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

The Evolution of Cannabis Analysis at the Canadian Border

Jaycee Fiering, Acting Senior Chemist, Canada Border Services Agency

10:45am EST - 11:00pm EST | 3:45pm GMT - 4:00pm GMT

The Impact of Cannabis Legislation on Crime Laboratories (sponsored)

Kristin Johndreau, Forensic Chemistry Site Supervisor, NMS Labs

II:00am EST - II:30pm EST | 4:00pm GMT - 4:30pm GMT

Cannabis 2.0

Ray Padilla – Executive Director/ Colorado Drug Investigators Association Matt Stoneberger- President/ Colorado Drug Investigators Association

II:30am EST - I2:00pm EST | 4:30pm GMT - 5:00pm GMT

Panel Discussion with All Presenters

1:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

The Impact of Cannabis Legislation on Crime Laboratories (NMS Labs Sponsored Workshop)



Thursday - January 25th, 2024

Forensic Intelligence

8:45am EST – 9:00am EST | I:45pm GMT – 2:00pm GMT

Welcome & Introduction

Program Chairs Simon Dunne & Maggie Tam

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Use of Internet Traces to Detect and Monitor Online Markets

Dr Marie Morelato, Centre for Forensic Science, University of Technology Sydney, Australia Dr Quentin Rossy, Ecoles des Sciences Criminelles, University of Lausanne, Switzerland

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

Using Optical Character Recognition Technology to Face the Challenge of Spotting Precursor Chemicals

Gina Leow (CBRNE Engineer from Home Team Science and Technology Agency)

10:00am EST - 10:15am EST | 3:00pm GMT - 3:15pm GMT

Analysis of Seized Drugs by Direct Ionization ASAP-MS (sponsored)

Emily Lee, Application Scientist, Toxicology and Forensics R&D, Waters Corporation

10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

Developing Frameworks for Illicit Drug Trend Analysis Using Ambient Ionization Mass Spectrometry Data from Forensic, Law Enforcement, and Public Health Data

Edward Sisco, Research Chemist, National Institute of Standards and Technology

10:45am EST - 11:00pm EST | 3:45pm GMT - 4:00pm GMT

High Throughput Solutions for Drug Identification (sponsored)

Richard Seitz, Business Development Manager, Bruker

11:00am EST - 11:30pm EST | 4:00pm GMT - 4:30pm GMT

FIDBID, Forensic Intelligence 'For Free' from Large Volume Ilicit Drug Screening

Prof dr Arian van Asten, van 't Hoff Institute for Molecular Sciences (HIMS) and CLHC, Faculty of Science, University of Amsterdam, Amsterdam, The Netherlands

II:30am EST - I2:00pm EST | 4:30pm GMT - 5:00pm GMT

Panel Discussion with All Presenters

1:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

How to Alleviate the Backlogs in Seized Drugs Analysis and Obtain a More Trustworthy Results at the Same Time? Modern MS Technology in Service of the Forensic Community (Bruker Sponsored Workshop)



Friday - January 26th, 2024

Emerging Technologies

8:45am EST - 9:00am EST | 1:45pm GMT - 2:00pm GMT

Welcome & Introduction

Program Chairs Simon Dunne & Maggie Tam

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Near-Infrared Technology for Portable Drug Testing

Mr Harrison Fursman (Centre for Forensic Science, University of Technology Sydney, 15 Broadway, Ultimo NSW 2007, Australia)

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

Effective Fentanyl Analog Screening Using LC-TIMS-TOF MS/MS

Francisco Fernandez-Lima, Florida International University

10:00am EST - 10:15am EST | 3:00pm GMT - 3:15pm GMT

Student Poster Award

10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

Field Forward Forensics: Triaging the Detection Challenge, as Applied to Fentanyl Laced Pills

Ashish Tripathi, Bruce King, Dan Carmany, Roberta Xega, Andrew Walz, Elizabeth Dhummakupt, Neal Kline, Erik Emmons, Phillip Wilcox, Emily D. Lockhart, Joseph S. Bozenko, and Jason Guicheteau

10:45am EST - 11:00pm EST | 3:45pm GMT - 4:00pm GMT

Low Energy Ionization of Nitazenes and Fentanyl Analogs Using a GC/QTOF (sponsored)

Kirk Lokits, Ph.D. GCMS Applications Scientist, Agilent Technologies

II:00am EST - II:30pm EST | 4:00pm GMT - 4:30pm GMT

Assessment of a Synthetic Drug Laboratory by SICRIT-HRMS

Maximilian Greif, M.Sc.; Institute for Analytical Research (IFAR), Hochschulen Fresenius gemeinnützige Trägergesellschaft mbH, University of Applied Sciences, Idstein, Germany and Federal Criminal Police Office, Forensic Science Institute, Wiesbaden, Germany

II:30am EST - I2:00pm EST | 4:30pm GMT - 5:00pm GMT

Panel Discussion with All Presenters

I:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

Direct Ionization - MS: How Can You Implement This in Your Daily Workflow? (Waters Corporation Sponsored Workshop)

2:15pm EST - 3:15pm EST | 7:15pm GMT - 8:15pm GMT

Fundamentals of using MassHunter Unknowns Analysis for the Forensic Chemist (Agilent Technologies Sponsored Workshop)



9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Adapting to Dynamic Illicit Drug Lab Operations in the United States

Dean Kirby, Senior Research Chemist, Drug Enforcement
Administration, Special Testing and Research Laboratory, Dulles, Virginia USA

Abstract: Illicit drug production in the United States is a dynamic process. In response to changing laws and drug consumption patterns, the types of clandestine drug laboratories encountered by law enforcement agencies is also constantly evolving. Due to the chemical nature of drug labs, a forensic chemist is a crucial component of the investigational team. This lecture will cover a variety of drug manufacturing operations, from cannabis extraction to complex chemical synthesis using unique precursors, and will discuss two decades of lessons learned by a DEA chemist to include topics of safety, evidence collection and sampling, research, analysis and court testimony.

- a) understand the critical role that the forensic scientist plays in complex illicit drug manufacturing cases.
- b) recognize the hazardous chemicals and processes used in clandestine drug laboratories.
- c) identify key items of evidence that should be collected and tested to support criminal prosecution.





9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

Visualizing Contamination from Drugs and Homemade Explosives

Matthew Staymates, National Institute of Standards and Technology

Abstract: This work reports on a new NIST effort that helps us understand the spread of contamination during the manufacturing of homemade explosive devices and illegal drug mixtures. We couple qualitative flow visualization techniques with quantitative chemical analysis techniques to help identify the generation, evolution, transport, and ultimate fate of trace contamination during these activities. The primary goal is to measure the mass of material on various surfaces that one would expect to find around the vicinity of manufacturing an HME device or illegal drug material.

The mock builds were performed in a residential house in Morgantown, West Virginia, owned by the West Virginia University Forensic Science Department (used for forensic science education purposes). Here, we could control variables such as material formulation, grinding and mixing techniques, and indoor ventilation systems (HVAC). We used laser light sheet illumination to visualize the production of massive amounts of airborne particulate contamination during specific mixing and grinding operations. Accompanying this was the use of custom air particle measurement systems that monitor the air for PM2.5 airborne particulates in real time. Finally, swabbing of various surfaces within the house was performed to measure the contamination levels at locations up to 20 feet away from the build, and in other rooms of the house.

This presentation will provide details of the mock builds, along with many flow visualization examples that demonstrate how this contamination is produced, along with how it transports through the house, and the amount of material we measured within the house. We will also have a partner poster during the poster session that discusses the details of the quantitative mass measurement techniques used, along with an interactive virtual-reality experience (using VR goggles) that allows you to be in the room during the mock build and look around at contamination levels and the changes in airborne particulate contamination in real time while the "bad guy" builds these illegal devices.

- a) Have a better understanding of how forensically-relevant contamination is generated and transported.
- b) Have a better understanding of how much contamination would be expected after manufacturing in a residential setting.
- c) Have a better understanding of how flow visualization techniques can be applied to a variety of forensic efforts and larger scientific pursuits.



10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

Clandestine Production Labs in the Netherlands a Daily Challenge

Dr. Sander Oldenhof, Drug Expert at the Netherlands Forensic Institute

Abstract: The clandestine production of (synthetic) drugs remains a big problem in the Netherlands. Historically the Netherlands is known for its production of amphetamine and MDMA, but in recent years the production of illicit drugs has diversified. Clandestine production locations of methamphetamine and extraction locations of cocaine are commonly encountered, as well as the production of other synthetic drugs e.g. cathinones. In this talk I will give some insight into 'just another day at the office' by showing some of the recent developments in the synthetic drug production in the Netherlands.

- a) know about the current state of illicit drugs production in the Netherlands.
- b) have gained insights into the production processes of several drugs as performed in the Netherlands.
- c) have learned what kind of investigations we perform on these kind of production locations.





10:45am EST - 11:00am EST | 3:45pm GMT - 4:00pm GMT

What's New on the Designer Drug Scene: Synthetic Cannabinoids, Precursors, and More (sponsored)

Holly Pierzynski, MS, Manager of Forensic Novel Psychoactive Substance Research, Cayman Chemical

Abstract: As an important partner to the forensic community, Cayman Chemical is dedicated to the research, development, and production of a wide variety of research/analytical tools. It is our responsibility to monitor current trends and rapidly develop reference standards necessary for the early detection of NPS. This presentation will discuss recent developments among several popular drug classes. We will cover new analogues that have appeared recently on the grey marketplace with an emphasis on synthetic cannabinoids (such as NMDMSB and MDMB-PICA). We will also review the emergence of synthetic precursors that are being sold for the non-legitimate production of opioids, benzodiazepines, and synthetic cannabinoids.

- a) Be familiar with the latest synthetic cannabinoids that are in circulation.
- b) Recognize the latest synthetic cannabinoid precursors and benzodiazepine prodrugs being sold on the illicit market and understand how they can be used to make several different NPS final products.
- c) Understand what precursors/impurities/adulterants are currently being seen in non-pharmaceutical fentanyl drug seizure samples.



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II:00am EST - II:30am EST | 4:00pm GMT - 4:30pm GMT

Clandestine Laboratory Trends and Challenges in Western Canada

Adrienne Law, Clandestine Laboratory Specialist, Drug Analysis Services Laboratory, Health Canada

Abstract: Health Canada's Drug Analysis Services (DAS) has three laboratories that serve Canada's various police agencies. The labs are located in Vancouver, Toronto, and Montreal. On average DAS receives around 120,000 exhibits annually across the three labs. Samples that are submitted to DAS are seized and sampled by the police officers, thus only a portion of the total exhibit is submitted.

The presentation will highlight the shift in the type and scale of clandestine drug labs encountered in BC and AB in the past 5 years. Recently encountered large scale fentanyl and MDMA synthesis labs will be detailed, with discussion on changes seen in the types of precursors used for each.

Some interesting challenges in clandestine drug lab response will also be covered.

- a) Become familiar with the clandestine laboratory trends in Western Canada.
- b) Become familiar with the synthesis routes for fentanyl and MDMA currently used.
- c) Know the scale and type of equipment we have seen consistently for both the fentanyl and MDMA clandestine labs.





I:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

Delving into the World of Lyseramides: The Past, Present, and Future (Cayman Chemical Sponsored Workshop)

Camille Watson-Gooden Ph.D., Scientist I, Forensic NPS Research Department, Cayman Chemical cwatsongooden@caymanchem.com

Danielle St. Germaine, Scientist II, Forensic Chemistry Department, Cayman Chemical dstgermaine@caymanchem.com

Abstract: Lysergamides are a class of alkaloids with a tetracyclic ergoline core structure. These compounds elicit their hallucinogenic properties by binding to and activating the serotonin 2A receptor. Variations to the ergoline core typically occur at three main regions of the core. These modifications give rise to some analogs with comparable efficacy to lysergic acid diethylamide (LSD). Join us and learn more about the history, modifications, fragmentation, and new emerging analogs of Lysergamides.

Detailed Learning Objectives:

- a) Be familiar with the history, pharmacology, common substitutions, and naming of Lysergamides.
- b) Be able to recognize common patterns and fragmentation pathways of Lysergamides to assist with
- f uture identifications.
- c) Have knowledge of most current emerging Lysergamides on the illicit market.

Camille Watson-Gooden is an experienced synthetic organic chemist in the Forensic NPS Research Department at Cayman Chemical. She earned her BS in Chemistry at the University of the West Indies, Mona Campus in Jamaica. She then earned her Ph.D. in Organic Chemistry at Michigan State University. Camille has been with Cayman since 2020 and her focus is on the research, development, and synthesis of emerging novel psychoactive substances.

Danielle St. Germaine is an experienced synthetic organic chemist in the Forensic Chemistry Department at Cayman Chemical. She earned her BS in Biochemistry and Toxicology as well as her MS degree in Chemistry at Eastern Michigan University. While at Cayman Chemical, she has worked in both the Medicinal Chemistry and Forensic Chemistry Departments. Danielle's current area





9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Australian Illicit Drug Trends and Profiling Insights

Ms Erin Ellis and Miss Kirra King – Australian Federal Police Forensic Drug Intelligence Analysts

Abstract: This presentation from the Australian Federal Police (AFP) will provide an overview of the current illicit drug trends observed at the Australian border, with a particular focus on drugs seizures from the Americas and Europe, from the perspective of the AFP's Forensic Drug Intelligence (FDI) team. FDI leads the Australian Illicit Drug Intelligence Program (AIDIP), which involves the collection of drug profiling information from AFP illicit drug seizures. Physical and chemical characteristics from these seizures are collated and subsequently assessed to provide operational and strategic insights on the international and national drug market impacting Australia.

In Australia, drug profiling is directed towards drug types commonly seized in large quantities at the Australian border including methamphetamine, cocaine and heroin. It is acknowledged that over the past few years' active collaboration between AFP and International Law Enforcement Agencies has played an important role in the disruption of drug trafficking to Australia from American and European countries. The sharing of forensic intelligence will further enhance this cooperation.

- a) Gain a deeper understanding of the Forensic Drug Intelligence capabilities within the AFP and Australia's Illicit Drug Intelligence Program (AIDIP).
- b) Gain greater insight to the current Australian illicit drug market and emerging trends.
- c) Better understand how forensic intelligence can be used to inform investigations and disrupt crime





9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

A Forensic Perspective to Chemical Profiling of Illicit Drugs

Sami Huhtala, Forensic Chemist, National Bureau of Investigation, Finland

Abstract: There is a clear increasing trend in the use of chemometrics (i.e. multivariate analysis and other statistical methods) in forensic laboratories. This can be seen in forensic literature covering such as drug profiling, but also in arson debris analysis, spectral imaging, glass analysis, age determination, and more. In particular, current chemometric applications cover spectral (i.e. FT-IR) and chromatographic (i.e. GC-MS) data. All this has created a need for reliable and structured interpretation and assessment of both analytical and chemometric results.

Seized material, like suspected illicit drugs, in police investigations raises legal questions to be answered regarding identity (classification) and origin of specimens (comparison). The type of question being asked determines the analytical process, data handling and interpretation needed.

Correctly formulated question to forensic laboratory is the most important element of the process. The use of chemometrics can help in answering to the question. Utilization of chemometrics may also provide additional information in complex crime cases. Once chemists have been acquainted with this and taught how to apply chemometrics, the next step is to provide an understanding of when it is necessary to go further and provide the classification and comparison with assessed uncertainties. The aim of the ongoing project is to continue the path started earlier and evolve it with a good understanding when and how LRs can be used. Only a limited number of forensic laboratories have capabilities to develop and apply chemometrics as well as do LR calculation. Producing LRs is highly context specific and easily falls out of the realm of strictly chemometrics.

The results and conclusions of forensic analyses need to be communicated in a comprehensible form and explained with sufficient clarity to investigative units and to the court of law in order to be used effectively. Ultimately, the forensic analysis must answer the original request presented by the investigative unit in clear and reliable way.

- a) perceive the role of chemometrics in forensic work flow
- b) develop a fine understanding of the potential uses of chemometrics in forensic chemistry
- c) be introduced to the assessment and reporting of forensic results



10:15am EST - 10:45am EST | 3:15pm GMT - 3:45pm GMT

DEA's Chemical Profiling - Drug Intelligence from the Lab

Joe Bozenko, Senior Research Chemist, DEA Special Testing & Research Laboratory

Abstract: The US Drug Enforcement Administration's Special Testing and Research Laboratory provides in-depth chemical analysis to support investigations and intelligence operations. Through cutting-edge technology and expansive reach throughout the world of illicit drugs, four programs comprising major drug threats to the United States have been developed. This presentation will cover the Signature Programs for Cocaine and Heroin as well as the Profiling Programs for Methamphetamine and Fentanyl. The evolution of these programs and the current state of information provided will be presented and discussed.

- a) The attendees will identify the extension of forensic chemistry to provide intelligence information on drugs through profiling.
- b) The attendees will be able to identify the requisites to produce intelligence products through signature and profiling.
- c) The attendees will be familiar with the limitations and expectations to both profiling and signature programs.





10:45am EST - 11:00am | 3:45pm GMT - 4:00pm GMT

Spectral Libraries for Detection & Identification of NPS (sponsored)

Tim Stratton, Manager Library Technologies, Thermo Fisher Scientific

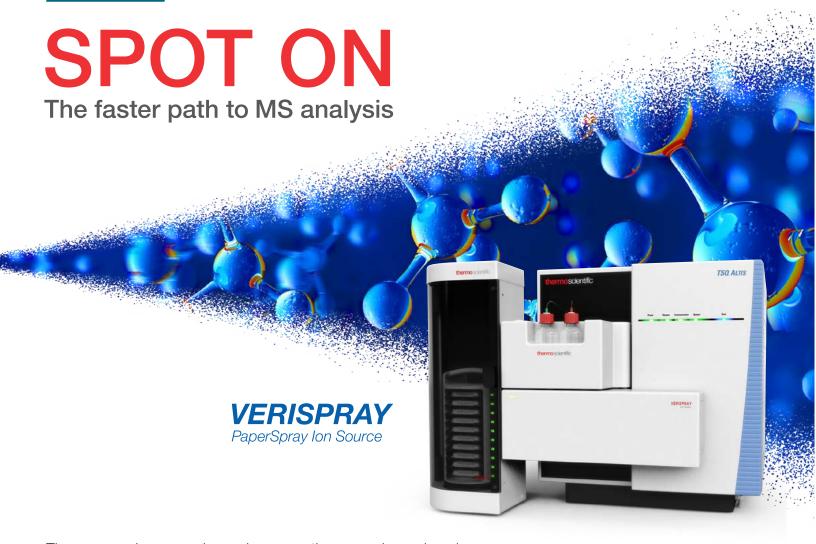
Abstract: Spectral libraries of reference compound data are a useful tool for the identification of compounds. Compound identification relies on having appropriate fragmentation data to provide the most confident spectral match. However, there will always be compounds that are not reflected in reference libraries such as newly synthesized compounds or compounds for which standards are not available, making identification via matching spectra impossible, even with optimal acquisition. A reference library can be utilized to educate our acquisition approaches across a wide range of structure classes. Reference spectral libraries can still provide a wealth of tools for the detection and potential identification of such unknown compounds. Spectral similarity searching can provide us with relevant potential hits that can be combined with orthogonal approaches such as molecular networking to highlight compounds of interest in complex samples. In addition, the reference library can provide a depth of fragments relevant to a group of structurally related compounds which can be used as a resource for finding candidates via class-based searching. We will discuss these approaches and more including approaches for de novo structure determination via substructure identification from MSn data.

- a) Identify optimal data acquisition strategies for confident compound identification
- b) Understand multiple library-based approaches to detecting unknown components of interest
- c) Be aware of the application of MSn data for substructure ID of unknown components of interest.





Toxicology



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II:00am EST - II:30am | 4:00pm GMT - 4:15pm GMT

Profiling in Real Time: Combining Chemical Correctness with Big Data Analysis

Simon Dunne, National Forensic Center (NFC), Swedish Police Authority, Sweden

Abstract: The study of impurity profiles for narcotics seizures can yield a plethora of information regarding synthetic routes, cutting agents, storage history and links to other seized materials. Taken together with indices such as chemical identity, concentration, packaging/stamp traits a complex web of data is amassed that needs thorough processing in order to provide forensic evidence. Whilst traditional profiling methods have relied heavily upon pairwise visual comparisons of GC-FID and GC-MS chromatograms, this approach is subjective and difficult to both quantify and document. The complex nature of the data leads itself naturally to the use of modern multivariate data analysis techniques to properly address the multidimensionality of the task.

Illicit preparations such as amphetamine, cocaine, cannabis hashish and heroin are not chemically inert, in that they contain solvent, reactants, volatile components and side products. During drying (often necessary before analysis) chemical changes to the impurity profile may occur due to evaporation, oxidation and pH-changes. An in-depth knowledge of the constituents of these profiles, their physiochemical properties, interrelationships and matrices is therefore essential for reliable comparative analyses.

Whilst the complexity of these analyses would seem to render them inappropriate for producing good strategic intelligence within an appropriate operative timeframe, NFC has generated a new quantitative and generic approach to chemical profiling that can significantly reduce case-handling times and subjectivity, whilst simplifying case documentation and strengthening scientific conclusions. Whilst most profiling methods utilize a limited selection of reference peaks from complex chromatograms, there are often many non-reference peaks which also contain significant information for comparative analysis but are not currently utilized in quantitative analysis. To capture this information NFC has initiated secondary holistic profiling methods which utilize the entire chromatogram for the assessment of similarity using both traditional distance measurements and Al-methodology totally free of peak definition or integration. The co-evaluation of both the reference peak profile and the chromatogram in its entirety (both analyzed automatically and free of subjectivity) generates strategic information within minutes for intelligence purposes or as a guide in detailed profiling analyses.

- a) Develop an understanding for the complexity and challenges involved in the comparative analysis of chemical profiles.
- b) Understand the need for non-subjective and quantitative analysis of chromatographic profiles.
- c) Understand the interplay between statistical and artificial intelligence methods in forensic comparative analysis.



I:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

Paper Spray Mass Spectrometry for Quantitative, High Throughput Drug Testing (ThermoFisher Sponsored Workshop)

Professor Chris G. Gill, Ph.D., P.Chem.

Co-Director, Applied Environmental Research Laboratories, Chemistry Department, Vancouver Island University, Nanaimo, BC, Canada.

Chemistry Department, University of Victoria, Victoria, BC, Canada.

Chemistry Department, Simon Fraser University, Burnaby, BC, Canada.

Department of Environmental and Occupational Health Sci., University of Washington, Seattle, WA, USA.

Canadian Institute for Substance Use Research, University of Victoria, Victoria, BC, Canada.

Abstract: The opioid overdose crisis in Canada has resulted in more unnatural deaths than all other causes. Mitigation strategies are being explored by a wide spectrum of partners, including governments and health agencies, in an attempt to reduce the societal, economic, and personal harms from illicit drug use. Drug checking has gained considerable interest and is demonstrating efficacy, allowing people who use drugs (PWUD) to submit samples of their illicit drugs for chemical analysis to receive information about the substance they intend to use. Paper spray mass spectrometry (PS-MS) is now in use by our group as a novel, on-site quantitative drug checking strategy, providing significantly increased selectivity, sensitivity and adaptability over existing on-site drug checking technologies. This work demonstrates quantitative, on-site PS-MS drug checking as a valuable tool for harm reduction in the opioid overdose crisis as well as illicit drug supply surveillance.

OBJECTIVES: To demonstrate the use and effectiveness of PS-MS as an on-site, rapid, quantitative drug checking strategy for harm reduction drug checking and illicit supply surveillance.

METHODS: Measurements were performed by paper spray tandem mass spectrometry with a highthroughput paper spray ion source (Thermo Scientific™ TSQ Fortis™ triple quadrupole mass spectrometer with a VeriSpray™ source). The quantitative method targets 105 drugs, and a full scan measurement identifies new substances. Small drug samples (~Img) submitted by PWUD are dissolved in methanol, diluted to within the calibration range, and then directly analyzed on-site in Victoria, BC, Canada, through a collaboration with the Vancouver Island Drug Checking Project. Presented data includes samples from January 2021-present. The time from sample submission to relaying results to a client is on the order of minutes.

RESULTS: PS-MS results from data collected for over 10,000 drug samples demonstrate that it shows excellent promise for drug checking. Less skilled personnel can successfully generate reliable PS-MS measurements. The method shows a high degree of sensitivity and selectivity (LLOQ < 0.01% in solids). We have detected the unexpected presence of trace levels of carfentanil and its synthetic analogs in illicit samples, and quantified the presence of a variety of novel benzodiazepines in >60% of illicit opioid samples. Alternative drug checking is also conducted: immunoassay test strips can detect the presence of fentanyl or related analogs, but lack the selectivity to explicitly detect the presence of potent drugs at trace levels such as carfentanil. Low active drug concentrations detected by PS-MS are frequently missed by FT-IR and Raman due to their inherently higher detection limits. Expected cocaine, methamphetamine, MDMA, and ketamine samples are generally not adulterated with other actives. However, opioid samples (fentanyl and/or heroin) are frequently adulterated with multiple actives. As an example, the detection of novel benzodiazepines (e.g. desalkylgidazepam) in opioid drugs highlights the strengths of the PS-MS method: the low levels quantified are frequently not detected by FT-IR, and benzodiazepine immunoassay strips are highly unreliable.

CONCLUSION: On-site drug checking by PS-MS for harm reduction is effective for use by less skilled harm reduction workers. The ability or provide rapid, sensitive and quantitative drug checking has also provided a comprehensive understanding of the high variability of the illicit drug supply composition. Providing rapid and accurate feedback to PWUD to inform better decisions regarding drug use (e.g. reducing dose or discarding dangerous substances) is a significant step forward in reducing harms from a toxic drug supply. PS-MS is presented as a powerful, front-line technology with demonstrated impact in harm reduction settings. Results inform PWUD and health care professionals alike,

providing oversight within a variable and unsafe drug supply.



Detailed Learning Objectives:

- a) What Paper Spray Mass Spectrometry (PS-MS) is.
- b) How a PS-MS workflow is being used for routine quantitative harm reduction and illicit drug supply surveillance in Victoria, BC.
- c) Advantages of direct mass spectrometry strategies such as PS-MS for the high throughput, quantitative measurements of illicit drugs.

Professor Chris G. Gill, Ph.D., P.Chem. Chris is a Chemistry Professor at Vancouver Island University. He conducts pure & applied research, developing direct mass spectrometry methods for measurements in complex samples. This has led to transformative environmental, industrial & clinical/bioanalytical measurement advances. Research interests include developing high precision systems and approaches for environmental & clinical diagnostics, forensic testing, & on-site drug testing strategies for harm reduction & supply surveillance.



I:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

Advances in Ambient Mass Spectrometry for the Rapid Analysis of Drugs of Abuse (ThermoFisher Sponsored Workshop)

Stefania Boccuzzi, PhD student, King's College London

Abstract: Mass spectrometry is a highly valuable analytical tool used in the field of toxicology, with untargeted and targeted applications for the analysis of drugs of abuse. Previously, our research group has demonstrated the benefits of liquid chromatography-high-resolution accurate mass systems for untargeted analyses of in vitro transesterification products of synthetic cannabinoids (SC) and in vitro metabolites of SC and synthetic cathinones (SCt). The next phase of our research focuses on using the latest ambient ionisation approaches for targeted triple-quadrupole applications in the form of paper spray ionisation (PSI). Based on electrospray ionisation mechanisms, PSI generates ions directly from a sample spotted onto a paper substrate. PSI uses dried matrix spots (DMS) which offer improved matrix stability due to fewer enzymatic processes taking place as a result of matrix dehydration. Using PSI and DMS combined eliminates the need for sample extraction or chromatography, leading to rapid results and lower cost per analysis compared with traditional techniques like liquid chromatography-mass spectrometry. Currently, we are investigating the stability of drugs of abuse in DMS by use of a VeriSpray™ PaperSpray Ion Source coupled to a TSQ Altis™ Plus Triple Quadrupole Mass Spectrometer. Short-term studies will determine whether DMS offer improved analyte stability of SCt compared with previous stability studies in liquid matrices, whereas long-term studies will investigate the stability of a wider drug panel in previously spotted and stored dried plasma spots compared with present-day spotting of the same samples. Our future work will centre around the analysis of plasma samples from patients presenting to an inner London emergency department (ED) with acute drug toxicity. Currently, clinicians rely on self-report and clinical patterns of toxicity to determine the drug(s) likely to be involved. Using the VeriSpray™ system for identifying and estimating the concentration(s) of drug(s) present in a patient sample has the potential to enable clinicians to tailor management early in the course of the ED presentation based on analytically confirmed drug use.

Detailed Learning Objectives:

- a) have an insight into how paper-spray mass spectrometry compares to traditional chromatographic techniques
- b) appreciate the advances that paper-spray mass spectrometry can bring for the rapid analysis of drugs of abuse
- c) gain insight into the importance of analytically confirming drug use in a patient experiencing acute drug toxicity

Stefania Boccuzzi, PhD student, King's College London Following my background in forensic science and toxicology, I began my PhD in Analytical Toxicology at King's College London in June 2022 which involves an exciting collaboration with Thermo Fisher Scientific for clinical toxicology applications. My PhD project focuses on the use of paper spray ionisation coupled to a triple quadrupole mass spectrometer for the analysis of plasma samples from patients who have presented to emergency departments experiencing acute drug toxicity.





Wednesday - January 24th, 2024

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

The Impact of Cannabis Legalization on Poisonings

Dr Rose Cairns, Senior Lecturer in Pharmacy, The University of Sydney; and Director of Research, New South Wales Poisons Information Centre, Sydney, Australia

Abstract: Many countries have moved to decriminalize or legalize medical and recreational use of cannabis in the past three decades. Medicinal cannabis legislation expands treatment options for conditions including refractory epilepsy, while recreational cannabis legislation aims to allow safe use while reducing criminal activity and use of other drugs including Synthetic Cannabinoid Receptor Agonists (SCRAs). However, these changes can also have negative public health impacts. With increasing use and availability of cannabis in the community comes the risk of harms, including overdose and poisoning. Cannabis can cause severe toxicity, particularly in children.

This presentation will summarize findings of a recently published systematic review that investigated the effect of cannabis legalization and decriminalization on poisoning. In addition, new Australian data on the impact of legalization of medicinal cannabis will be presented. The clinical effects of cannabis poisoning will be summarized.

The systematic review of four databases examined cannabis/cannabinoid poisoning exposures following legalization and decriminalization of medicinal and recreational cannabis. This revealed 30 studies meeting inclusion criteria, with data available from the US, Canada and Thailand. Most studies (n=19) investigated pediatric poisoning. Most studies (n=24) reported an increase in poisonings, however the magnitude varied greatly. Our pooled estimate indicated an increase in poisoning after legalization (RR: 3.56, 95% CI: 2.43-5.20), which was greater in studies that focused on pediatric patients (RR: 4.31, 95% CI: 2.30-8.07). When compared with legalization of flower-based products and oils, legalization of commercial sales of "edibles" was associated with increased poisoning exposures and hospitalisations, particularly in children.

New data from Australia's largest poisons information center shows a steady increase in cannabis poisoning exposures following legalization of medicinal cannabis in 2016. Exposures increased by 15.3% per year (95% CI: 12 to 18% per year, P < 0.001). Pediatric exposures were increasing at the fastest rate. There is a need for better poisoning data to quantify the impact of cannabis legalization globally. While many countries have changed cannabis legislation, the vast majority of published data comes from North America. Future studies should account for time-varying confounders and consider preintervention trends using robust experimental design.

Risks from poisoning should be considered by any jurisdiction that is considering changing access to cannabis. In particular, the risk of pediatric poisoning from cannabis edibles should be recognized. Not legalizing commercial sales of edibles is one strategy. Risk could also be mitigated with poisoning prevention measures including opaque packaging and child resistant closures.

- a) Understand the impact of cannabis legalization on poisonings from available data in the US, Canada, Thailand and Australia.
- b) Describe clinical features of cannabis and synthetic cannabinoid receptor agonist (SCRA) toxicity, including differences in adult and pediatric toxicity.
- c) Describe the poisoning risk posed by cannabis "edibles" and public health/poisoning prevention strategies to mitigate this.



Wednesday - January 24th, 2024

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

The EU Market for Cannabis: Increasing Complexity Poses Higher Risks to Users' Health and Challenges to Policymakers

Laurent Laniel, principal scientific analyst, markets, crime and supply reduction, EMCDDA

Abstract: Cannabis is the largest illicit drug market in the EU. While overall stable in terms of numbers of users (22.6 million in 2021), the market is now much more complex and dynamic than in the past. Some of the changes that took place over the last 5 years are likely to have increased health risks for users. This is partially a result of the increasing availability of a broader range of consumer products based on a wider variety of natural, semi-synthetic and synthetic cannabinoids, while the delta-9-THC content of herbal and resin products appears to have increased dramatically. Routes of administration available to cannabinoid consumers have also become more varied and in addition to the long-standing practice of smoking, now more frequently include vaping, "dabbing" and eating. An increase in products containing highly potent, dangerous synthetic cannabinoids has also been noted, a concerning development since these may be mi-sold to consumers as based on natural cannabinoids.

Domestic cannabis production in the EU is significant and appears to cover an important proportion of regional consumer demand often after being smuggled using complex patterns of trafficking routes within the EU. However, large amounts of cannabis resin and herbal cannabis continue to be smuggled from regions outside the EU such as Morocco and the Western Balkans, while synthetic cannabinoids are mostly sourced in China. North America seems to have emerged quite recently as a source of several types of products available in Europe, including herbal cannabis, and e-liquids and edible products containing natural or semi-synthetic cannabinoids. Several of the products smuggled into Europe from North America appear to have been commercially manufactured in jurisdictions where cannabis has been legalised for recreational use, while other products may be counterfeit versions of those.

A simultaneous development has been the emergence of a range of low-THC cannabis products for different consumer uses, such as foods and cosmetics. Some products focus on health and well-being, while others appear to mimic products on the illicit market. Overall, products containing extracts of the cannabis plant are appearing across a range of commercial sectors under different regulatory frameworks. In some cases, this has caused confusion surrounding their legality.

While the cannabis market in the EU is changing, important developments in cannabis policy are simultaneously taking place. This includes a ruling by the Court of Justice of the European Union (CJEU) in November 2020, clarifying that CBD does not currently fall within the scope of narcotic control laws when interpreting EU laws. Czechia, Germany, Luxembourg, Malta and the Netherlands have proposed or implemented new policies or experiments related to cannabis for recreational use. Developments regarding cannabis are unfolding rapidly and creating complex challenges for policymakers and other stakeholders, such as potential tensions and blurred boundaries between the regulatory approaches used in commerce, medicine and drug control.

- a) Better understand recent changes in the EU cannabis market, some of their public health implications and the challenges that arise for policy-making and monitoring
- b) Be aware of key trends in EU cannabis retail markets and consumer products based on the last data and information available at European level
- c) Be aware of key production and supply trends based on the last data and information available at European level



Wednesday – January 24th, 2024 10:15am EST – 10:45am EST | 3:15pm GMT – 3:45pm GMT

The Evolution of Cannabis Analysis at the Canadian Border

Jaycee Fiering, Acting Senior Chemist, Canada Border Services Agency

Abstract: The cannabis group at the Canada Border Services Agency (CBSA) laboratory is the team responsible for analyzing suspected cannabis samples. Our group was developed as a result of cannabis legalization in Canada and how this led to a need for more sensitive and quantitative methods. We have two main clients, with different analysis needs, the first being CBSA itself and the second being Canada Revenue Agency (CRA). Our work for CBSA includes the analysis of samples seized at the borders and mail centers that require complex analysis in order to make a determination on the presence or absence of cannabis or industrial hemp. Additionally, we quantitatively analyze cannabis samples for CRA to aid with their enforcement of the Excise Act 2001 and the collection of excise taxes on cannabis products sold within Canada.

The legalization of cannabis in Canada in 2018 has driven the cannabis group to develop new extraction methods and improve the analysis methods within our laboratory, and it continues to drive us to improve our capabilities and streamline our cannabis analysis workflow. Regarding sample extraction, cannabis products can come in many forms, including plant material, oils, concentrates, and a variety of edible and topical products (eg; soft candy, chocolate, cookies, bath bombs, shampoos, and creams). Due to this fact, we have had to develop a wide variety of extractions in order to clean up these samples prior to analysis. We are also working to improve our instrumentation methods, which currently include GCMS and LC-MS/MS, to improve sensitivity and robustness as a way to better support the Border Service Officers and Excise Officers in their enforcement of cannabis legislation.

These points will be discussed further in this presentation, along with some general trends observed in Canada since cannabis legalization, and some techniques that we believe will improve and streamline cannabis analysis in the future.

- Learn what the cannabis section currently does when analyzing cannabis samples in the context of legalization.
- b) Understand the challenges that have been faced when moving into quantitative analysis and what has been done to overcome these challenges.
- c) Hear about what methods/analyses the cannabis section will be working on developing in order to further improve and streamline our cannabis sample workflow.



Wednesday - January 24th, 2024

10:45am EST - 11:00pm EST | 3:45pm GMT - 4:00pm GMT

The Impact of Cannabis Legislation on Crime Laboratories (sponsored)

Kristin Johndreau, Forensic Chemistry Site Supervisor, NMS Labs

Abstract: The passing of the 2018 Federal Farm Act and the legalization of marijuana in many states has changed how crime laboratories approach the testing of marijuana and marijuana-related samples. The testing has become more complex and reporting language can be confusing. The cannabinoid market has also grown, introducing a large variety of samples to the lab that bring new challenges to sample preparation and data analysis interpretation. This saturated market has also led to an increase in these sample types being received at lab. With hemp being defined as containing 0.3% or less of decarboxylated delta-9-THC (total delta-9-THC), laboratories must be able to reliably differentiate between the different THC isomers.

- a) Understand the impact legalization has had on how hemp/marijuana testing is conducted
- b) Understand the importance of THC isomers and how we distinguish them in the laboratory
- c) Understand the evolution of sample types and how they can introduce new challenges to the laboratory





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Don't miss "The Impact of Cannabis Legislation on Crime Laboratories"

January 24, 2023 | Presentation 10:45 AM - 11:00 AM Eastern | Workshop 1:00 PM - 2:00 PM Eastern



Wednesday - January 24th, 2024

II:00am EST - II:30pm EST | 4:00pm GMT - 4:30pm GMT

Cannabis 2.0

Ray Padilla – Executive Director/ Colorado Drug Investigators Association Matt Stoneberger- President/ Colorado Drug Investigators Association

Abstract: With the legalization of recreational cannabis in Colorado in 2012, the State has become ground zero for the recreational cannabis movement. Despite common public misconceptions that the industry is properly regulated and cannabis is medically beneficial, Colorado cannabis has become a highly lucrative way to funnel millions of dollars into criminal organizations which has further escalated crime and produced societal decay. This presentation will discuss what has occurred 11 years following cannabis legalization to include the following:

- Normalization of cannabis in Colorado
- Arguments for and against legalization
- Current US cannabis landscape
- · Cannabis related traffic fatalities
- · Cannabis related to impaired driving
- Youth. Adult Use of cannabis
- Social Media
- Hospital/ ER/ Poison Control issues
- Black market and organized Crime
- Escalating crime rates
- Butane Hash Oil Explosions and Risk
- Homelessness

- a) Have an understanding of the impacts of cannabis legalization in the United States
- b) Have an understanding of cannabis in relation to traffic fatalities, impared driving and poison control in Colorado
- c) Have an understanding of the risks associated to cannabis edibles, concentrates and the danger of production by use of butane hash oil extractions



Wednesday - January 24th, 2024 1:00pm EST - 2:00pm EST | 6:00pm GMT - 7:00pm GMT

The Impact of Cannabis Legislation on Crime Laboratories (NMS Labs Sponsored Workshop)

Kristin Johndreau, Forensic Chemistry Site Supervisor, NMS Labs

Abstract: Over the past five years, many states have adopted more lenient legislation for marijuana use, that has impacted crime laboratories and their testing approaches. The passing of the 2018 Federal Farm Act and the legalization of marijuana in many states has changed how crime laboratories approach the testing of marijuana and marijuana-related samples. The cannabinoid market has also grown, introducing a large variety of sample types to the lab that bring new challenges to sample preparation and data analysis interpretation. The combination of the large variety of sample types with various definitions of marijuana has increased testing and reporting complexities.

Three (3) Detailed Learning Objectives: After having attended this presentation, one will

- a) How to navigate federal and State definitions for hemp vs marijuana.
- b) Understand the importance in the increase in the number of measurable THC isomers and how we distinguish them in the laboratory.
- c) Understand the evolution of sample types and how they can introduce new challenges to the laboratory including the breadth and depth of variation of vapes and sample types for hemp/marijuana.

Kristin Johndreau, Forensic Chemistry Site Supervisor, NMS Labs Kristin Johndreau has a BS in Genetics from University of California, Davis and a MS in Forensic Science from Arcadia University. She has worked for NMS for over 9 years in Forensic Drug Chemistry and has worked at 5 of their 6 locations. She is a certified chemist by the Maryland Department of Health and holds a forensic analyst license in seized drugs from the Texas Forensic Science Commission.





Thursday - January 25th, 2024

9:00am EST - 9:30am EST | 2:00pm GMT - 2:30pm GMT

Use of Internet Traces to Detect and Monitor Online Markets

Dr Marie Morelato, Centre for Forensic Science, University of Technology Sydney, Australia Dr Quentin Rossy, Ecoles des Sciences Criminelles, University of Lausanne, Switzerland

Abstract: Online platforms have reshaped legal business models and influenced illicit trade similarly. By examining publicly accessible internet traces left on marketplaces, forums, and review websites alongside traditional market descriptors, forensic science can effectively monitor illicit markets and uncover insights about the activities behind them. This presentation aims to explain how detecting and monitoring online convergence settings sheds light on the dynamics and structure of the online drug and doping product markets. It showcases results from multiple studies focused on detecting online shops, monitoring trends on forums, and search engine queries on the web. Furthermore, since illicit drugs and doping substances are tangible products, combining digital, physical, and chemical traces is crucial for a complete market analysis. We will present results from test purchases, demonstrating how physical/chemical analysis of these products validates hypotheses drawn from online indicators and connects online activities to physical locations. These studies demonstrate that internet traces are an invaluable and complementary source of information that can be used to understand illicit drug markets. In addition, they may help monitor emerging threats. It is suggested that the forensic analysis of internet traces should be adopted more systematically.

- a) appreciate the significance and complementary nature of internet traces in detecting and monitoring illicit drug markets
- b) recognise that integrating digital, physical, and chemical traces produces offers a more holistic view of the market
- c) understand how the detection and monitoring of online sources provide insights into the characteristics and evolution of the online illicit market, including its structure





Thursday - January 25th, 2024

9:30am EST - 10:00am EST | 2:30pm GMT - 3:00pm GMT

Using Optical Character Recognition Technology to Face the Challenge of Spotting Precursor Chemicals

Gina Leow (CBRNE Engineer from Home Team Science and Technology Agency)

Abstract: The driving factor behind this innovation to create this mobile application was to improve the efficiency of the ground officers in identifying and reporting of substances during their operations. Currently at the borders, officers would have to manually go through manifests declaration, MSDS and labels on goods to check if the cargo contain any items of interest such as explosive precursor. When suspicious items are being identified, officer would use the internet to help them identify or find out more of the materials, this takes up much time of the officer. Last but not least, officers would have to do a manual reporting of the detection to their supervisor or team. This is challenging for officer as not there are such a large pool of security sensitive material. The development of this mobile application aims to assist the officer in the identification of substances and the reporting when such items of interests are detected at the borders. The app helps to significantly reduce the time taken to identify material of interest as it focuses on a specific list of material of interest. New material of interest can also be added to the app when require.

Incorporating databases and technologies such as Optical Character Recognition (OCR) and Computer Vision (CV) into a mobile application allows for a more digitalized and automated workflow in a compact form factor. Officers will be able to swiftly capture photos of labels and extract text via OCR and key visual information using CV. The mobile application facilitates automation by searching the embedded databases to determine if the text extracted contains any materials of interest via a matching algorithm and generates a report in a set template with details such as date and time already pre-filled. Through the mobile application, officers can obtain more details about the items of interests, such as their other known names, appearances, and incompatibles of such items. It is designed to be a custom-fit solution that takes advantage of the ubiquity of smart devices to be incorporated into the different daily operations of officers without disruption – it can be installed on smartphones or tablets alike. The mobile application allows for the customization of the database with the substances of interest relevant to each agency, periodic updates with newly popular or emergent substances, and supports offline usages as the algorithms are installed locally on the smartphones. These app has many potential applications including enforcement in homeland and border security.

- a) Learn about the potential of incorporation of technology to increase workflow efficiency
- b) Understand the importance of design centric thinking in creating solutions
- c) Understand how garnering support and willingness to iteratively trial solutions will help with the refinement of the application



Thursday - January 25th, 2024 10:00am EST - 10:15am EST | 3:00pm GMT - 3:15pm GMT

Analysis of Seized Drugs by Direct Ionization ASAP-MS (sponsored)

Emily Lee, Application Scientist, Toxicology and Forensics R&D, Waters Corporation

Abstract: The analysis of seized drugs plays a vital role in the effectiveness of national and international programs which aim to control the use, trafficking, and distribution of illegal drug substances. However, the sheer number of samples received for analysis, places a huge burden on the drug control laboratories and drug enforcement agencies. The increase in number, diversity, and potential toxicity of drugs with the continued emergence of potent novel psychoactive substances (NPS) also presents significant challenges for drug control laboratories to keep their screening methods up to date with all compounds of concern. Typical workflows include colorimetric tests, FTIR, or TLC presumptive screening analysis followed up by confirmatory analysis using gas chromatography in combination with mass spectrometry (GC-MS). However, for many drugs, colorimetric tests are not available or result in a high rate of false positives, FTIR results of mixtures can be

inconclusive and TLC analysis can be time consuming. This can lead to more samples requiring analysis by GC-MS leading to sample bottlenecks and backlogs. Therefore, methods that can facilitate a fast, but accurate, screening of drugs are of interest. The aim of this study was to assess the potential of RADIAN™ ASAP Mass Detector, a compact device based on Atmospheric Solids Analysis Probe-Mass Spectrometry (ASAP-MS), as a simple, yet rapid, screening tool for seized materials.

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- How direct ionization mass spectrometry can be used to rapidly screen seizures for drugs
- The mechanism of ASAP ionization and its suitability for rapid screening for drugs
- Sample preparation and analytical methodology for common drugs and NPS





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Thursday – January 25th, 2024 10:15am EST – 10:45am EST | 3:15pm GMT – 3:45pm GMT

Developing Frameworks for Illicit Drug Trend Analysis Using Ambient Ionization Mass Spectrometry Data from Forensic, Law Enforcement, and Public Health Data

Edward Sisco, Research Chemist, National Institute of Standards and Technology

Abstract: Understanding trends in the illicit drug landscape is an area of active research for many due to the potential forensic intelligence information that can be obtained. The ability to actively detect and make sense of changes in the drug landscape can provide insight into drug trafficking patterns and assist in dismantling drug distribution networks. It can also provide critical insight for public health entities who can stage overdose prevention resources proactively, instead of reactively.

While there are many types of data that can be used to understand the landscape, our work focuses on monitoring changes and trends based on a materials chemical signature. To obtain near real-time information, we have employed ambient ionization mass spectrometry (AI-MS) for rapid, comprehensive analysis of samples. This approach not only increases the volume of samples that can be analyzed per instrument but also provides a method capable of analyzing both bulk and residue samples with minimal sample pretreatment.

In this talk, current efforts to leverage Al-MS data from multiple sources (forensics, public health, and law enforcement) will be discussed. The development of statistical tools and algorithms to collate these chemical signatures and unlock insights into the drug landscape for different geographical regions in the United States will be highlighted. How we combine this data with additional meta data (i.e., type of paraphernalia or packaging) to further understand trends in the drug landscape will be highlighted. Ongoing efforts to build out predictive modeling to anticipate changes in the drug supply will also be discussed. Finally, the impact this information has had on our collaborative partners, both from the law enforcement and, more importantly, the public health communities will be presented.

- a) gain insight into ongoing efforts to develop near real-time trend analysis tools.
- b) learn how merging data from multiple analytical techniques can be accomplished.
- understand the role that ambient ionization mass spectrometry can serve in the illicit drug analysis workflow.



Thursday – January 25th, 2024 10:45am EST – 11:00pm EST | 3:45pm GMT – 4:00pm GMT

High Throughput Solutions for Drug Identification (sponsored)

Richard Seitz, Business Development Manager, Bruker

Abstract: Bruker manufactures mass spectrometers and software suited for analysis of incoming goods, seized drugs, and unidentified substances in support of the forensic and security communities. As part of the discussion, we will introduce solutions that provide the ability to accurately confirm the identify of known substances while maintaining the ability to retrospectively screen the same data for enhanced interrogations of a sample. TargetScreener is a complete solution of hardware, software, methods, and libraries designed to work with any of our high resolution QTOF mass spectrometers. By acquiring ion mobility measurements with our timsTOF platform, TargetScreener 4D provides additional identification criteria through the incorporation of Collisional Cross Section (CCS) values. CCS values are a property of a given molecule and can be used as a data point for both quality control and structural confirmation.

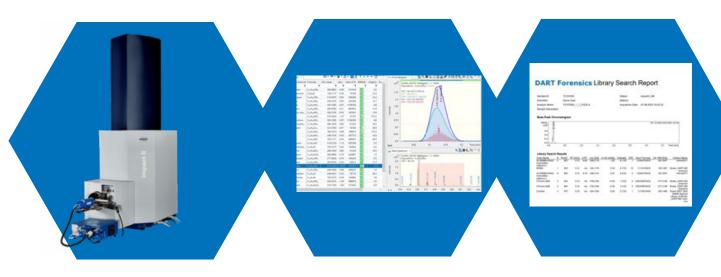
The need for rapid analysis is becoming more of a demand and is critical in providing the ability to adapt quickly to reactive situations where confident identifications are critical. Our incorporation of the DART ion source into the Bruker portfolio along with our focus on building DART-MS specific applications is enabling more complete solutions to the field for both targeted and non-targeted investigations. During the discussion there will be a few examples of screening and quantitation with DART-HRMS and introduce the first fully integrated system the EVOQ DART-TQ+.

- a) Understand Bruker's Mass Spec Solutions for Forensics and Drug ID -Bruker Confidential
- b) Understand the Basics of TargetScreener and TargetScreener 4D with CCS integration
- c) Gain an introduction to Bruker's emphasis on DART-MS for speed in identification and quantitation.





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- Less Maintenance
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Aquisition

Analysis

Reporting



Thursday - January 25th, 2024 11:00am EST - 11:30pm EST | 4:00pm GMT - 4:30pm GMT

FIDBID, Forensic Intelligence 'For Free' from Large Volume Ilicit Drug Screening

Prof dr Arian van Asten, van 't Hoff Institute for Molecular Sciences (HIMS) and CLHC, Faculty of Science, University of Amsterdam, Amsterdam, The Netherlands

Abstract: The primary objective of the FIDBID (Forensic Illicit Drug Intelligence through Big and Intelligent Analysis of Chemical and Criminological Data) initiative is to unearth, extract, and leverage valuable insights concealed within the daily chemical data generated in the illicit drug screening processes. Forensic laboratories routinely analyze physical evidence (powders, pills, liquids, blotter paper) for the presence of drugs of abuse using GC-MS. Presently, this wealth of information remains untapped due to the intense focus on managing the substantial caseload and the need to rapidly report the identification of listed hard and soft drugs.

Within the FIDBID consortium, forensic illicit drug experts, criminologists, and data scientists collaborate to create real-time insights into illicit drug market dynamics by identifying impurities, adulterants, and other trace compounds. The presence of such trace compounds holds crucial significance in understanding the production, origin, and smuggling of the evidence material. Through the application of advanced big data-processing and analysis tools, this chemical information will automatically emerge from the vast volume of data generated in thousands of cases each year without affecting the primary process.

The subsequent step involves transforming this supplementary chemical information into valuable intelligence. This process ncorporates case-specific forensic details and a comprehensive criminological comprehension of the criminal networks engaged in illicit drug-related activities in the Netherlands. By facilitating accessible and practical entry to this wealth of information, derived from 'big-chem-data,' through professional, tailor-made interfaces, the FIDBID project seeks to equip the criminal justice system and the Dutch government with innovative tools. These tools will enhance their capacity to comprehend, impede, and combat drugrelated subversive activities strategically and on a case-by-case basis, both within the Netherlands and internationally.

- a) acquire a deep understanding of the FIDBID project, including its primary objectives, challenges in current forensic analysis, and the untapped potential within chemical illicit drug GC-MS data.
- b) gain insight into the collaborative approach between forensic experts, criminologists, and data scientists within the FIDBID consortium, and understand how their combined expertise enhances the extraction of valuable chemical information for investigative purposes.
- c) develop awareness of the practical applications of FIDBID-derived intelligence in law enforcement, including the automation of chemical data analysis, the transformation of data into actionable intelligence, and the strategic utilization of this information to combat illicit drug-related activities.



Thursday – January 25th, 2024 1:00pm EST – 2:00pm EST | 6:00pm GMT – 7:00pm GMT

How to Alleviate the Backlogs in Seized Drugs Analysis and Obtain a More Trustworthy Results at the Same Time? Modern MS Technology in Service of the Forensic Community (Bruker Sponsored Workshop) William Fatigante, Application Scientist Bruker Applied Mass Spectrometry

Abstract: For many forensic labs persistent backlogs in seized drugs analysis continue to be the bane of their existence. Growing influx of new synthetic drugs and stringent requirements of court evidence acceptance make this problem that much more challenging. A remedy for this ongoing struggle may be found in adoption of modern, yet already proven technologies and workflows.

The use of Direct Analysis in Real Time in conjunction with High Resolution Mass Spectrometry (DARTHRMS) as a forensic tool has been praised for its ability to generate reliable analytical results much faster and easier than alternative techniques. However, a critical missing element was a complete single-vendor solution backed by a trusted database of analytes and capable of automating the entire workflow from sample introduction to report generation. Bruker Applied Mass Spectrometry has bridged this gap by acquiring the DART technology, integrating it with its HRMS instruments and developing an automated workflow based on the trusted NIST library of illicit drugs for DART analysis. Running samples and generating reports in seconds instead of tens of minutes is no longer just a feasibility, but a practical, reliable, and cost-effective option.

Furthermore, the combination of DART and HRMS technologies can now be expanded to separate and accurately identify even isomers of various drugs. This becomes possible with addition of Trapped Ion Mobility Spectrometry (TIMS) stage in the HRMS instrument that allows for measurement of Collisional Cross Section (CCS), or simply put - the sizes of the molecules of interest. In combination with accurate mass, isotopic pattern, and ion fragmentation data, this information can be used to identify previously unknown NPS such as new synthetic cannabinoids, fentanyl analogues, or other completely unknown compounds.

While the main area of interest often lies with identifying unknown analytes, the ability to gather any additional information is also important to forensic practitioners. Using the speed and simplicity of DART analysis with the discernability of TIMS-enabled HRMS (timsTOF), it becomes possible not only to detect these analytes of interest but begin to classify possible sources of origin for similar sample types. This instrumentation working powered by Bruker non-targeted analysis software, can quickly sift through complicated datasets both identifying analytes and visualizing relevant information using supervised and non-supervised statistics, such as PCA and t-test.

All these workflows and underlying technologies will be explained and illustrated with real life examples through the course of this presentation.

William Fatigante, Application Scientist Bruker Applied Mass Spectrometry William Fatigante is an applications scientist within the applied markets division of Bruker, concentrating on DART related applications. He received his Master of Science from Illinois State University where he focused on applying ambient mass spectrometric methods for forensic evidence screening and confirmation. Being with Bruker now for almost a year, William has learned the ins and outs of DART-MS and its potential to provide a rapid screening solution to the ever-present sample backlog within the forensic community.



FAST

Seized Drug Screening with DART-MS and NIST Library

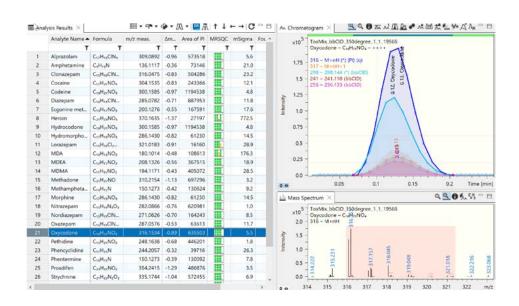
Established technique and trusted library in a well supported out-of-the-box package

- Chromatographic screenings are time consuming and prone to maintenance issues
- Newer illicit drugs are being abused and transported in unprecedented volumes
- Gases and solvents are expensive and environmentally unfriendly

High sample backlogs can be reduced and difficult drug identifications can be improved by using Bruker's DART/MS platform. Minimal sample preparation, rapid analysis, and library search reports within seconds.

- Samples per minute vs samples per hour
- Improved turn around time







Friday – January 26th, 2024 9:00am EST – 9:30am EST | 2:00pm GMT – 2:30pm GMT

Near-Infrared Technology for Portable Drug Testing

Mr Harrison Fursman (Centre for Forensic Science, University of Technology Sydney, 15 Broadway, Ultimo NSW 2007, Australia)

Abstract: The prevalence and availability of illicit drugs within Australia continue to be pervasive and dynamic. Within 2020-21, a record amount of drug seizures, in both weight (41.4 tonnes) and number (n=105,694), were recorded nationally across a variety of illicit drugs [1]. The capacity to rapidly identify and quantify illicit drugs is paramount to removing their availability from the drug supply chain within Australia. In the past, accomplishing this has faced challenges with regard to the expense, speed of analysis, accuracy and quantity of information provided by previous in-field techniques [2]. Nearinfrared (NIR) spectroscopy combined with chemometric modelling has proven to overcome these limitations in order to provide robust qualitative and quantitative information on a suspected illicit substance in real time [3]. This study aimed to investigate portable NIR spectroscopy and develop chemometric models for an Australian context to evaluate its potential in the rapid identification and quantification of illicit drugs.

Testing and chemometric model development was undertaken using illicit drug seizures captured from various sources (including traditional domestic crime scene and international mail specimens) by the Australian Federal Police (AFP). The seizures selected for sampling were diverse in terms of purity and separated into calibration and validation datasets to appropriately train the chemometric models. NIR spectra were collected using the MicroNIR (Viavi Solutions Inc.) connected to the NIRLab infrastructure (https://nirlab.com/) and compared to reference laboratory analysis conducted on the same specimen by gas chromatography – mass spectrometry. Three illicit drugs were focused upon; cocaine and heroin (to validate chemometric models developed by the University of Lausanne [3] for Australian implementation) and methamphetamine (related to its popularity within Australia).

Various NIR spectra were collected across the aforementioned illicit drugs (n=612). In terms of identification, NIR spectroscopy has demonstrated high sensitivity and specificity for the chemometric models tested (accuracy > 95%). For the quantification, the predicted purities provided by the NIR technology were accurate and mostly fell within the acceptable uncertainty (+/- 15%). The potential broader implementation of this portable analytical instrumentation will be discussed. It is argued that it would not only greatly support frontline policing in terms of investigative and intelligence-led decisionmaking but also the health and well-being of people. Furthermore, NIR spectroscopy can be integrated into current testing protocols effortlessly, could help reduce significant casework loads within forensic laboratories and enable the reprioritisation of laboratories on more difficult substances (such as new psychoactive substances or complex mixtures).

Detailed Learning Objectives:

- understand the potential of near-infrared spectroscopy and chemometric modelling for illicit drug identification and quantification
- recognise the importance of decentralising the forensic laboratory to increase efficiency in a world of ever-decreasing resources
- experience the potential of this technology to be integrated operationally to increase safety, efficiency and informed decision-making at the frontline policing

References:

- 1. Australian Criminal Intelligence Commission, Illicit drug data report 2020-21. 2023, Commonwealth of Australia: Canberra, Australia.
- 2. Liu, C.-m., Han, Y., Min, S.-g., Jia, W., Meng, X., and Liu, P.-p., Rapid qualitative and quantitative analysis of methamphetamine, ketamine, heroin, and cocaine by near-infrared spectroscopy. Forensic Science International, 2018. 290: p. 162-168.
- 3. Coppey, F., Bécue, A., Sacré, P.-Y., Ziemons, E.M., Hubert, P., and Esseiva, P., Providing illicit drugs results in five seconds using ultra-portable nir technology: An opportunity for forensic laboratories to cope with the trend toward the decentralization of forensic capabilities. Forensic Science International, 2020. 317: p. 110498.



Friday – January 26th, 2024 9:30am EST – 10:00am EST | 2:30pm GMT – 3:00pm GMT

Effective Fentanyl Analog Screening Using LC-TIMS-TOF MS/MS

Francisco Fernandez-Lima, Florida International University

Abstract: We have previously shown the advantages of trapped ion mobility (TIMS) coupled to TOF for detection and separation of isomeric opioids. In this work, we further study the analytical separation capabilities of TIMS, in tandem with liquid chromatography and tandem MS/MS. In addition, atmospheric pressure sources (API) that enable high throughput and minimal sample preparation are effective for rapid scans of fentanyl analogs. Results will demonstrate the analytical power of complementary analytical separation to achieve low limits of detection (< Ippb) as well as the potential of API variants for the rapid screening over 230 fentanyl analogs. The influence of the ionization method on the mobility and ms profiles will be discussed.

- a) Demonstration of isomeric separation of fentanyl analogs based on their mobility in LC time scales
- b) high dynamic range of LC-TIMS-TOF MS/MS workflows and low limits of detection
- c) Advantages of API-TIMS-MS for direct and rapid screening of fentanyl containing surfaces





Friday – January 26th, 2024 10:15am EST – 10:45am EST | 3:15pm GMT – 3:45pm GMT

Field forward forensics: Triaging the Detection Challenge, as Applied to Fentanyl Laced Pills

Ashish Tripathi¹, Bruce King¹, Dan Carmany², Roberta Xega¹, Andrew Walz¹, Elizabeth Dhummakup¹, Neal Kline¹ Erik Emmons¹, Phillip Wilcox¹, Emily D. Lockhart³, Joseph S. Bozenko₃, and Jason Guicheteau¹

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³Special Testing and Research Laboratory, Drug Enforcement Agency, Sterling, VA, USA

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Abstract: For the defense community trying to develop detection capabilities for military, security, and emergency response forces, the current and future strategic environment means that there are literally thousands of lethal materials that can be used as weapons. The sensing of chemical threats is important to obtain "real-time" answers that allow actionable decisions to be made on-the-spot; to reduce the logistical burden by moving the analysis closer to the source of the sample; to rapidly screen materials to identify samples that need to be sent to a lab for additional analysis and minimize the number of these samples; and to nondestructively analyze large, valuable, or immovable objects for which excising samples is not possible. This presentation details a multi-team approach to triaging trace threat materials through rapid orthogonal technologies to ascertain forensic level information, closer to the point of origin. Discussed will be the development of a portable Raman microscopy system allowing the noninvasive, non-destructive analysis of various types of surfaces and samplers for initial contamination determination. Samplers could consist of consumables already associated with other techniques, for example, mass spectrometry or ion-mobility swabs utilized at checkpoints, screening locations, and sensitive site exploitations. The swabs can be used in typical fashion to swipe a surface, but before being inserted into the mass spec or IMS, which are chemically destructive techniques, Raman microscopy can be performed to determine initial chemical contamination. Samplers could also consist of modified paper based substrates which contain chemical coatings to enhance interaction of the potential threat. In this particular scenario, a surface-enhanced Raman spectroscopy (SERS) substrate coated with gold or silver nanoparticles, can be analyzed by a portable Raman system. The same substrate could then be analyzed by the portable Raman microscope for additional information, and finally analyzed by a portable mass spectrometer yielding three individual data points within a matter of minutes all on the same sample. We will demonstrate the triage methodology in detecting fentanyl in fake oxycodone pills confiscated by US law enforcement agencies.



Friday – January 26th, 2024 10:45am EST – 11:00pm EST | 3:45pm GMT – 4:00pm GMT

Low Energy Ionization of Nitazenes and Fentanyl Analogs Using a GC/QTOF (sponsored)

Kirk Lokits, Ph.D. GCMS Applications Scientist, Agilent Technologies

Abstract: Identifying fentanyl analogs and other types of illicit drugs such as nitazenes, under the standard 70 eV ionization energy, can generate similar or non-specific spectral patterns between analogs that can differ structurally or vary in molecular weight. During this 15-minute segment you will learn about low energy ionization techniques to reduce the difficulty of identifying compounds with similar El spectra by producing a molecular ion utilizing low energy (10- 20 eV) ionization. This can result in an enhanced level of confidence during analyte identification and improve spectral certainty based on isotopic fidelity and ion fragment stability in a low energy ionization environment.

- a) Understand how low energy ionization works on a HR-GCMS-QTOF.
- b) Learn the capabilities of low energy ionization to form molecular ions of compounds that generate similar spectra.
- c) Learn how to combine compound HR Mass spectral data in combination with molecular ion generation, RT, and RT penalties to assist in compound screening and identification





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Friday – January 26th, 2024 11:00am EST – 11:30pm EST | 4:00pm GMT – 4:30pm GMT

Assessment of a Synthetic Drug Laboratory by SICRIT-HRMS

Maximilian Greif, M.Sc.; Institute for Analytical Research (IFAR), Hochschulen Fresenius gemeinnützige Trägergesellschaft mbH, University of Applied Sciences, Idstein, Germany and Federal Criminal Police Office, Forensic Science Institute, Wiesbaden, Germany

Abstract: With the ongoing trend towards large-scale amphetamine production in Europe, the output of clandestine laboratories is expanding. As synthetic drug production creates a tremendous amount of chemical waste, typically several tons of different types of production waste and other samples stored in numerous containers need to be characterized after seizure of a clandestine laboratory to assess its production features and scale and draw conclusions on potentially produced batches. Aim of this work is to evaluate the suitability of the SICRIT® (soft ionization by chemical reaction in transfer) ion source in combination with high-resolution mass spectrometry in an ambient mass spectrometry approach for rapid classification of samples from a seized clandestine drug laboratory for amphetamine production via the Leuckart route after pre-precursor conversion. A commercial SICRIT ion source was coupled with a QToF system and reference substances as well as synthesis waste samples were positioned in front of the inlet for data acquisition. High-resolution mass spectra were extracted and processed in RStudio. By using reference substances, target compounds like amphetamine, precursors (benzyl methyl ketone), reaction intermediates (N-formylamphetamine) and by-products (e.g., 4-methyl-5-phenylpyrimidine) could be identified in general in the mass spectral data. Many compounds were not only detected as [M+H]+ but as a variety of ion species per compound (e.g., [M+xO+H]+), which were identified by correlation plots and confirmed by fragmentation. Besides identification of target substances by headspace analysis of seized samples it was also possible to group related samples by cluster analysis. Based on these promising results, several machine learning algorithms were evaluated for generation of a classification model for assessment of unknown samples. In general, headspace analysis of various samples from a seized largescale clandestine amphetamine laboratory using the SICRIT - high-resolution mass spectrometry approach proved to be successful for classification and characterization of seized samples. The obtained results indicate the suitability of this methodology and its future potential.

- know a novel ion source for ambient ionization mass spectrometry methods
- know that samples from clandestine synthetic drug laboratories can be rapidly characterized by ambient ionization mass spectrometry
- c) have got an idea of the potential of machine learning algorithms in forensic sciences



Friday – January 26th, 2024 1:00pm EST – 2:00pm EST | 6:00pm GMT – 7:00pm GMT

Direct Ionization - MS: How Can You Implement This in Your Daily **Workflow? (Waters Corporation Sponsored Workshop)**

Emily Lee, Application Scientist, Toxicology and Forensics R&D, Waters Corporation John Vukovic, Clinical LCMS Account manager, Waters Corporation Rachel Lieberman, Global Forensic and Toxicology Marketing Manager, Waters Corporation

Abstract: The analysis of seized drugs plays a vital role in the effectiveness of national and international programs which aim to control the use, trafficking, and distribution of illegal drug substances. Typical workflows include colorimetric tests, FTIR, or TLC presumptive screening analysis followed up by confirmatory analysis using gas chromatography in combination with mass spectrometry (GC-MS). However, for many drugs, colorimetric tests are not available or result in a high rate of false positives, FTIR results of mixtures can be inconclusive and TLC analysis can be time consuming. This can lead to more samples requiring analysis by GC-MS leading to sample bottlenecks and backlogs. In this workshop we will dive into the details of Direct ionization MS and how the RADIAN™ ASAP Mass Detector, a compact device based on Atmospheric Solids Analysis Probe-Mass Spectrometry (ASAP-MS), could be used for a screening tool for seized materials. You'll learn about seized drug applications, how our customers currently use the instrument and get a chance to ask your questions.

For forensic use only.

- Learn how direct ionization mass spectrometry can be used to rapidly screen seized drugs
- b) The mechanism of ASAP ionization and its suitability for rapid screening for drugs
- Have the opportunity to ask questions regarding this direct-MS technique





Friday – January 26th, 2024 2:15pm EST – 3:15pm EST | 7:15pm GMT – 8:15pm GMT

Fundamentals of using MassHunter Unknowns Analysis for the Forensic Chemist (Agilent Technologies Sponsored Workshop)

Kirk Lokits – Agilent Technologies GCMS Applications Scientist

The I-hour workshop is designed to introduce the audience to the workflows involved when using Unknowns Analysis in the MassHunter software. The workshop begins with a 10-minute explanation of the deconvolution process, differences between deconvolution and peak integration, and some of the variables involved when using this powerful data analysis tool. Running through workflows, utilizing forensic data, the session will illustrate how to translate established workflows within MSD ChemStation Data Analysis to MassHunter Unknowns Analysis. The workshop will include how to generate an inhouse library in Unknowns Analysis, how to link retention time and or retention indices to each library entry and apply these entries to increase your Library Match Score (LMS) confidence level. Examples of Unknowns Analysis reporting templates will be demonstrated from the workshop exercises.





Dean Kirby

Senior Research Chemist, Drug Enforcement Administration, Special Testing and Research Laboratory, Dulles, Virginia USA

Mr. Kirby came to forensics following a 14-year career as a Medicinal Chemist at the Salk Institute for Biological Studies in La Jolla, California where he was involved in the design and synthesis of novel drug candidates. In 2002, Mr. Kirby joined the Drug Enforcement Administration's Southwest Laboratory in Vista, CA. Mr. Kirby has analyzed thousands of drug exhibits, and has testified as an expert witness over 50 times in both federal and state courts. Further, Mr. Kirby's work often takes him out in the field where he has investigated numerous clandestine drug laboratories attempting to produce various psychoactive substances and is often called as an expert to consult with investigators and attorneys when complex chemistry is involved. Mr. Kirby has provided instruction to thousands of domestic and international law enforcement and military personnel, specifically on the challenges of safely processing synthetic products and precursor chemicals found in clandestine laboratory environments. More recently, Mr. Kirby's career has come full circle when joined the organic chemistry team at DEA's Special Testing and Research Laboratory in the role of Senior Research Chemist and Technical Leader of the Fentanyl Profiling Program.

Matthew Staymates

National Institute of Standards and Technology

Matthew Staymates is a mechanical engineer and fluid dynamicist at the National Institute of Standards and Technology (NIST). His research interests focus on improving trace drug and explosives detection systems, developing next-generation detection technologies, and advancing forensic chemistry with scientific visualization. His expertise is in advanced fluid flow visualization and flow diagnostic techniques, including schlieren and shadowgraphy, highspeed imaging, and laser sheet flow visualization.





Dr. Sander Oldenhof

Drug Expert at the Netherlands Forensic Institute

After finishing a PhD in homogenous catalysis/organic chemistry at the University of Amsterdam I came into contact with forensic chemistry during my postdoc at the University of Delft/ Netherlands Forensic Institute (NFI). In 2017 I joined the illicit drugs team at the NFI where I currently am one of the forensic expert in the field of illicit drug production.



Holly Pierzynski, MS

Manager of Forensic Novel Psychoactive Substance Research, Cayman Chemical

Holly Pierzynski is the Manager of the Forensic NPS Research Department at Cayman Chemical. Holly is an experienced synthetic organic chemist with a BS in Biochemistry from Central Michigan University and a MS in Chemistry from Eastern Michigan University. Holly has been with Cayman since 2010 and the department she manages is tasked with the synthesis of novel psychoactive substance (NPS) reference standards. A main focus of Holly's work is tracking emerging NPS trends and the use of El-MS fragmentation analysis in collaboration with the forensic community toward the discovery of novel substances. She has presented her work at several forensic conferences.

Adrienne Law

Clandestine Laboratory Specialist, Drug Analysis Services Laboratory, Health Canada

Adrienne Law is a clandestine laboratory specialist with Health Canada's Drug Analysis Service (DAS) Laboratory located in Vancouver. She has been employed with the DAS lab for 20 years and has been in the specialist position for 7 years. Adrienne has a Bachelor's Degree in Chemical Engineering and a Bachelor of Technology in the Chemical Aspects of Forensic Investigation. She has attended more than 60 clandestine laboratories and has provided reports on 30 clandestine lab cases. Some of the labs she has attended include methamphetamine via red phosphorous and hypophosphorous, MDA, MDMA, fentanyl synthesis via Seigfreid, Valdez and Gupta, and a fentanyl milling operation. Adrienne has been an active member, board member and is currently the past president of the Clandestine Laboratory Investigating Chemists (CLIC) Association and has attended and presented at the annual training seminars since 2017.





Ms Erin Ellis



Miss Kirra King

Ms Erin Ellis & Miss Kirra King

Australian Federal Police Forensic Drug Intelligence Analysts

Erin Ellis and Kirra King are members of the AFP Forensic Drug Intelligence (FDI) team and have been since 2018 and 2020 respectively. During this time, they have produced technical drug intelligence to support AFP operations and create greater opportunities for prevention and disruption of crime. They also assist in the coordination of the AFP's drug profiling capabilities, which play a key role in defining a holistic overview of Australia's drug market.



Sami Huhtala

Forensic Chemist, National Bureau of Investigation, Finland

Forensic Chemist with broad experience in analytical chemistry related to pharmaceuticals and illicit drugs, chemical profiling and statistics, as well as environmental forensics.

Currently working as a case coordinator at the Forensic Laboratory of the Finnish National Bureau of Investigation.

Joe Bozenko

Senior Research Chemist, DEA Special Testing & Research Laboratory

Joe Bozenko is a Senior Research Chemist with the DEA's Special Testing and Research Laboratory at Dulles, Virginia and a Scientific Advisor to DEA's Special Operations Division. He's been with the DEA for 23+ years and investigates synthetic drug manufacturing around the world and has testified many times in Federal Court as a Subject-Matter Expert. Mr. Bozenko has processed some of the largest methamphetamine laboratories in the world, traveled extensively, and has authored and presented many reports and peer-reviewed scientific articles pertaining to the clandestine synthesis and analysis of controlled substances. In addition to this, Mr. Bozenko has also been instrumental in the development of the DEA's High-Hazard Level 'A' Clandestine Laboratory Response Training Program. Mr. Bozenko is closely involved with science-related officer safety and leads DEA's handheld instrumentation testing and evaluation. Mr. Bozenko is also charged with the specialized analysis of selected fentanyl, methamphetamine, and MDMA samples, both domestic and international, for intelligence purposes. Mr. Bozenko holds both Baccalaureate and Master's Degrees in Chemistry and is an Adjunct Professor of Chemistry at Shepherd University, a. Mr. Bozenko also holds a patent, jointly with Harvard University, on the Archimedes Magnetic Levitation System. Mr. Bozenko has been featured on television, periodicals, podcasts, and in Sam Quinones' new book The Least of Us: True Stories of American and Hope in the Times of Fentanyl and Meth.







Tim Stratton

Manager Library Technologies, Thermo Fisher Scientific

Tim Stratton joined Thermo Fisher Scientific 15 years ago in the pharmaceutical vertical marketing team. Tim has led the fragmentation spectral library project within Thermo Fisher Scientific that led to the creation of mzCloud and several library related acquisition, creation, and advanced search techniques. Prior to joining Thermo, Tim was a pharmaceutical research scientist where he specialized in metabolite and impurity structure determination.

Simon Dunne

National Forensic Center (NFC), Swedish Police Authority, Sweden

Simon Dunne is a forensic specialist working at the National Forensic Centre within the Swedish Police Authority. As the research coordinator for the Drug Analysis section Simon's work focusses upon methods for the detection and identification of new psychoactive substances, semi-automatic methods for chemical profiling of narcotics, the use of hyperspectral NIR imaging for determination of the identity and homogeneity of narcotics seizures, together with rapid screening using non-destructive spectroscopic techniques combined with tandem applications of unsupervised/supervised chemometric methods.





Dr Rose Cairns

Senior Lecturer in Pharmacy, The University of Sydney; and Director of Research, New South Wales Poisons Information Centre, Sydney, Australia

Dr Rose Cairns is a senior lecturer in pharmacy at the University of Sydney and is Director of Research at the New South Wales Poisons Information Centre. She is a Senior Research Fellow of Australia's National Health and Medical Research Council (NHMRC). She works clinically as a poisons information specialist, providing advice to healthcare professionals and the public. Her research in clinical toxicology focuses on poisoning prevention, in particular the impact of legislative changes on poisoning.





Laurent Laniel

Principal Scientific Analyst, Markets, Crime and Supply Reduction, EMCDDA

Laurent Laniel was trained as a translator and social scientist in France Spain and the UK, specializing in illicit drugs, geopolitics and security issues. He has done field work on drug production, trafficking, and control measures in Africa, the Americas, Asia and Europe. Before joining the EMCDDA in 2008, he worked as a researcher for Unesco and the French interior ministry. His last publication is "Captagon: déconstruction d'un mythe", Drogues, enjeux internationaux, n° 10, OFDT, Paris. X: @narcoexperto

Jaycee Fiering Acting Senior Chemist, Canada Border Services Agency

Jaycee Fiering is an Acting Senior Chemist in the Alcohol, Tobacco and Cannabis section of CBSA, working with the cannabis group. Her work includes the analysis of cannabis casework samples, as well as running a LC-MS/MS for the analysis of cannabis samples. She is also currently working on a project to verify a new method for cannabinoid quantification using LC-MS/MS. She completed her Bachelor of Science in Forensic Science and her Master of Science in Forensic Science degrees at Trent University.





Kristin Johndreau
Forensic Chemistry Site Supervisor, NMS Labs

Kristin Johndreau has a BS in Genetics from University of California, Davis and a MS in Forensic Science from Arcadia University. She has worked for NMS for over 9 years in Forensic Drug Chemistry and has worked at 5 of their 6 locations. She is a certified chemist by the Maryland Department of Health and holds a forensic analyst license in seized drugs from the Texas Forensic Science Commission.



Ray Padilla

Executive Director/ Colorado Drug Investigators Association

Ray Padilla is a Task Force Officer assigned to the DEA Rocky Mountain Division Financial Investigations Group and is primarily focused on organized crime associated with marijuana, money laundering and fentanyl investigations. During his more than 26 years in law enforcement, Ray has spent time as a patrol deputy and patrol sergeant for the Summit County Sheriff's Office in Breckenridge, Colorado and has spent the past 21 years with the Westminster Police Department in Westminster, Colorado, with assignments in Patrol, motorcycle enforcement and the North Metro Task Force, a multi- jurisdictional narcotics task force in north Denver, Colorado. Ray has been involved in narcotics enforcement for the last 14 years and has conducted hundreds of narcotics investigations, including several multi-year, Title III investigations focused on marijuana trafficking and organized crime.

Ray teaches both nationally and internationally and is recognized as an expert regarding narcotics / marijuana investigations. Ray is currently the Executive Director of the Colorado Drug Investigators Association and Co-Founder of Blue Vudu Training.

Matt Stoneberger

President/ Colorado Drug Investigators Association

Matt Stoneberger is an Agent-in-Charge with the Colorado Bureau of Investigation (CBI) and assigned to the CBI's Special Investigations & Illicit Marijuana Unit, Denver Team. Before CBI, Matt started his career with the Parker Police Department (Colorado) and, later worked as an investigator for the 18th Judicial District Attorney's Office (Colorado). After several years as a patrol officer, Matt began a variety of plain-clothes detective assignments. In his 23 years as a peace officer, Matt has spent the last 16 years as a dedicated narcotics detective. He has completed tours in the Douglas County Sheriff's Office Pattern Crimes Unit, South Metro Drug Task Force, DEA Denver Enforcement Group I, and the 18th Judicial District's Drug/Gang Unit. Matt has conducted hundreds of felony drug investigations, including domestic and international, multi-year, Title-III wiretap investigations targeting drug trafficking organizations. Matt has operated as an undercover 45+ times and participated in hundreds more undercover drug operations in various other capacities.



Matt is considered an expert in marijuana trafficking investigations and teaches both nationally and internationally regarding narcotic/ marijuana investigations.

Matt is the President of the Colorado Drug Investigators Association and Co-Founder of Blue Vudu Training.



Dr Marie Morelato

Centre for Forensic Science, University of Technology Sydney, Australia

Dr Marie Morelato is a senior lecturer and the course director of the Bachelor of Forensic Science at the Centre for Forensic Science, University of Technology Sydney. Her research involves the use of forensic case data in an intelligence perspective.





Dr Quentin Rossy Ecoles des Sciences Criminelles, University of Lausanne, Switzerland

Ass. Prof. Quentin Rossy leads the Masters in Crime Data Analysis and Traceology, focusing on crime analysis (online frauds and illicit markets) at Lausanne's School of Criminal Justice. His research focuses on the analysis of online serial crimes.

Gina Leow CBRNE Engineer from H

CBRNE Engineer from Home Team Science and Technology Agency

Gina Leow is a CBRNE Engineer with Home Team Science and Technology Agency, Singapore, working in the area of Technology scanning and analytics to augment Home Team Department in Singapore with the science and technology capabilities. As an engineer, Gina's work focusses on innovation, leveraging on technology and software development, for detection of concealed threat in parcel, baggage, and cargo. Her work also includes supporting home team with the implementation of technologies. Gina's work in borders security contributes to the interception of threats that also directly contribute to Homeland security.





Emily LeeApplication Scientist, Toxicology and Forensics R&D,
Waters Corporation

Emily Lee is an Application Scientist at Waters Corporation and is part of a global team dedicated to the development of forensic and toxicology applications. Prior to joining Waters, Emily worked in forensic toxicology laboratories in the UK where she gained experience in many aspects of day-to-day laboratory operations including sample extraction, analysis, method development and validation, analytical trouble shooting and reporting. Emily has a MSc in Forensic Science (Toxicology) from the University of Huddersfield.





Edward Sisco

Research Chemist, National Institute of Standards and Technology

Ed Sisco is a research chemist within the Surface and Trace
Chemical Analysis Group at the National Institute of Standards and Technology (NIST). His research focuses on addressing measurement challenges in forensic chemistry, public health, and law enforcement, developing next-generation measurement capabilities to address the opioid epidemic, and lowering implementation barriers for new technologies in the illicit drug detection arena.

Richard Seitz

Business Development Manager, Bruker

Richard is a life-long resident of Virginia and holds a BS in Chemistry from Old Dominion University. He has over 25 years of laboratory and instrumentation experience and he has spent a major portion of his career supporting technologies enabling the detection and analysis of chemical warfare agents and hazardous vapors. Now with Bruker's Applied Mass Spectrometry Division, his primary responsibilities are focused on supporting solutions for the forensics and toxicology markets.





Prof dr Arian van Asten

van 't Hoff Institute for Molecular Sciences (HIMS) and CLHC, Faculty of Science, University of Amsterdam, Amsterdam, The Netherlands

Prof. Arian van Asten joined the van 't Hoff Institute for Molecular Sciences of the University of Amsterdam (UvA) in 2012 on a special chair in Forensic Analytical Chemistry while working for the Netherlands Forensic Institute (2006-2018). In 2018, he transferred to the UvA and was appointed full professor in Forensic Analytical Chemistry and On-Scene Chemical Analysis. His research interests include the chemical profiling of explosives and drugs, the analysis of (bio)markers of CWA exposure, rapid chemical identification at the crime scene with portable instruments, the forensic use of comprehensive 2D chromatography, chemical imaging of forensic traces, and the use of data science to create forensic chemical intelligence. With Prof. Maurice Aalders he is responsible for the CLHC, the Netherlands Center for Forensic Science and Medicine. Additionally, he is the program director of the Master Forensic Science of the UvA. Prof van Asten has (co-)authored over 70 peer-reviewed scientific publications on (forensic) analytical chemistry, In 2023 his first academic book on forensic chemistry, entitled 'Chemical Analysis for Forensic Evidence', was published by Elsevier.





Mr Harrison Fursman

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Harrison is a PhD Candidate within the Centre for Forensic Science at the University of Technology Sydney. Harrison is currently working on optimizing a portable drug testing device that uses nearinfrared spectroscopy and chemometric modelling. He also is conducting a longitudinal chemical analysis of used syringes from the Sydney supervised injecting facility in order to obtain objective information on the drugs being injected there.

Francisco Fernandez-Lima

Florida International University

Dr. Francisco Fernandez-Lima is a Professor in the Department of Chemistry and Biochemistry at Florida International University. He is the recipient of a K99/R00 Pathway to Independence Awards by the National Institute of General Medical Sciences and a CAREER Award by the National Science Foundation. Since he joined FIU in 2012, he has published over 100 peer-reviewed research articles. He is the director of the "FIUMASS: MS experience for all" outreach program, FIU Mass Spectrometry Program and the President of the FIU Hispanic Faculty Association.





Kirk Lokits, Ph.D. GCMS Applications Scientist, Agilent Technologies

Kirk received his B.S. in Forensic Science and Chemistry from EKU and began his forensic tenure at the Miami Valley Regional Crime Laboratory in Dayton, Ohio and FDLE in the Orlando and Pensacola laboratories. Kirk left the forensic realm and began his career with HP/Agilent, working as a service engineer supporting the LC, GC, LCMS, GCMS, and ICPMS products. While working for HP Kirk earned his M.S. in Analytical Chemistry from MTSU. In 2005 Kirk left Agilent to attend the University of Cincinnati and earned his Ph.D. in Analytical Chemistry. Afterwards, he worked for the Midwest Research Institute (MRIGlobal) in Kansas City, as a Principal Chemist and Sr. Program Manager on DoD projects, staffing, designing, and building remote laboratories for placement throughout the world. In 2014, Kirk re-joined Agilent as a GCMS Applications Scientist focusing on forensic applications within the GCMS product line.





Maximilian Greif, M.Sc.

Institute for Analytical Research (IFAR), Hochschulen Fresenius gemeinnützigenTrägergesellschaft mbH, University of Applied Sciences, Idstein, Germany and Federal Criminal Police Office, Forensic Science Institute, Wiesbaden, Germany

Maximilian Greif graduated at Hochschule Fresenius in 2020 and worked at said university for one year as research assistant in the Horizon 2020 project SYSTEM. Since 2021, he is a joint PhD student at Hochschulen Fresenius and at the Forensic Science Institute of the Federal Criminal Police Office and since this time hen is also working part-time as lecturer at the same university. His research focuses on analytical chemistry applied to forensic sciences, especially to synthetic drugs.



Common Adulterants Trend In Illicit Heroin Seized In India And Its Forensic Relevance

Diksha Thakur, Research Scholar, Maharshi Dayanand University, Rohtak, Haryana Dr Rajvinder Singh, Associate Professor, Maharshi Dayanand University, Rohtak, Haryana Dr. Neeti Prakash Dubey, Additional Director, Regional Forensic Science Laboratory, Mandi, Himachal Pradesh

Abstract: Diacetylmorphine (DAM), is a semi-synthetic opioid that is frequently abused, particularly in Northern Region states like Punjab, Himachal Pradesh, New Delhi, Delhi-National Capital Region (NCR), Haryana, and Rajasthan. Tracking the precise source or trafficking networks is still daunting for law enforcement agencies. Here, forensic intelligence is essential for executing strategic and tactical actions. It is a well-established fact that DAM is illicitly synthesized in a clandestine laboratory. Various inherent or deliberately added adulterants/ contaminants were reported by various authors in their research studies. The motive behind adding the adulterants (diluents/cutting agents) to a pure drug sample is monetary benefits by increasing its quantity. Such impurities drastically impact the abuser's health, even death, due to overdose and synergistic impacts of chemical substances added to heroin. Each lot of confiscated consignments of Chitta has a unique chemical signature. Forensic chemical profiling concerning special impurities, contaminants, and adulterants can provide essential information about drug trafficking networks. The presence of these chemical substances varies at each step within the trafficking network. The universally accepted fact is that each offender has a peculiar modus operandi. This peculiar pattern of adding adulterants to illicit drug samples can aid in tracing the trafficking route and further dismantling its source. This poster tries to identify the common adulterants of illicit heroin in different regions. For this purpose, the authors utilize their personal forensic laboratory experience and scientific research studies conducted by other experts. Also, the significance of such adulterants in narrowing down the possible suspects and further dismantling the source and the network is explained. Furthermore, the loopholes existing in ongoing geographical profiling-based research studies are also highlighted. The author's recommendations and implications need to be implemented for dismantling the illegitimate network, and in the future geographical profilingbased research studies to build a comprehensive view are also represented.





A New, Rapid GCMS Addition to the NZ Customs/ESR Border Screening Laboratory at Auckland Airport, New Zealand

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Matthew Russell and Erina Mayo (Senior Scientist) The Institute of Environmental Science and Research

Craig Aitcheson (Technical Engineer) Agilent Technologies Ltd

Abstract: New Zealand Customs (Customs) and The Institute of Environmental Science and Research (ESR) Ltd work together screening consignments entering New Zealand through the international mail stream at Auckland Airport. The Customs/ESR Screening Laboratory began as a Proceeds of Crime funded project in 2014, to address the time-consuming and costly process of screening suspicious items seized at the border, along with the growing incidences of novel psychoactive substances (NPS). Although the laboratory's success during this period was well recognised, new challenges in the identification of minor and concealed components exposed some limitations in the detection capability of the current instrumentation (mainly Raman-based devices and FTIR) deployed at the border. Along with the associated false positives and negatives, these techniques have struggled to sufficiently address mixture resolution and have failed to identify minor, low dose, potentially harmful, components. Statistical outputs showed that the CESL laboratory had established the content of only 24% of samples in 2020 (down from 42% in 2015), with the rest being returned as either †negative or †unknown.

A project to scope and identify a technique that would address these issues coincided with Agilent's press release on its new QuickProbe for GCMS (QP-GCMS); a rapid analytical instrument requiring minimal sample preparation. The ESR-funded project included the analysis of approximately 700 samples, obtained from border intercepts, that were either mixtures of unidentified components or drug types that often produce weak or spurious results using the current techniques. These problematic matrices included organic/plant-based materials, cosmetics, oils, aqueous liquids, gels, paper tabs and tablets. Upon identification of a drug component, using conventional GCMS procedures, the sample was subsequently analysed by QP-GCMS with promising results. After resolving some

chromatographical challenges during method development, the QP-GCMS has since been successfully integrated into the border workflow, screening those substances that are not identified using Raman and FTIR. In the months since operation began in June 2022, approximately 650 samples have been analysed with an additional 48 compounds in 102 samples identified, equating to approximately 15% improvement in the identification of illicit substance in border seizures.





alpha-Methyltryptamine Metabolite Profiling in Humans

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Abstract:

Background and Aim

Product seizures, intoxications, and fatalities involving tryptamines are expected to rise due to the recent enthusiasm for psychedelics in therapeutics. alpha-Methyltryptamine (alpha-MT) is a synthetic tryptamine and novel psychoactive substance (NPS) that became popular for recreational use in the 2000s. alpha-MT abuse and/or seized material was reported in nine countries to date, and it was involved in several overdose fatalities in the United States and Europe. Detecting alpha-MT and/or metabolite biomarkers of consumption in biological matrices is therefore critical in forensic sciences to document intake. However, there is currently no data on alpha-MT metabolism in humans. The aim of the study was the determination of optimal metabolite biomarkers of alpha-MT consumption in human hepatocyte incubations and authentic postmortem samples.

Methods: First- and second- generation metabolites of alpha–MT in humans were predicted in silico with BioTransformer open-access software (v.3.0). alpha–MT was incubated with cryopreserved 10-donor-pooled human hepatocytes and sample analysis was performed with reversed-phase liquid chromatography (biphenyl column) coupled with high-resolution tandem mass spectrometry (LC-HRMS/MS) operated in positive- and negative-ionization modes; LC-HRMS/MS raw data were processed with Compound Discoverer (Thermo Scientific) for data mining, alpha–MT metabolites were identified in postmortem urine (with and without enzymatic hydrolysis) and blood from an alpha–MT fatal overdose using the same LC-HRM/MS analysis and data mining workflow.

Results: Nine metabolites were identified in vitro and eight additional metabolites were identified in urine (seventeen in total); only five metabolites identified in urine were also identified in blood due to the excretion of phase II metabolites. The main metabolic transformations were hydroxylation, O-sulfation, O- and N-glucuronidation, and N-acetylation at the indole core, consistent with the metabolism of structural analogues. Oxidative deamination, a major detoxification pathway of N,N-dimethyl tryptamines, was not detected in the present experiments, likely due to the methyl group protective effect, suggesting that co-administration of a monoamine oxidase inhibitor is unnecessary to induce psychedelic effects. Except for N-acetylation, all reactions were predicted in silico.

Conclusions: The use of psychedelic tryptamines is increasing, emphasizing the importance of laboratory identification of specific metabolite biomarkers to verify intake and identify potential public health outbreaks. We suggest alpha—MT, hydroxy-alpha—MT glucuronide, and two hydroxy-alpha—MT sulfates as biomarkers of alpha—MT use in non-hydrolyzed urine; we suggest alpha—MT, two hydroxy-alpha—MT sulfates and N-acetyl-alpha—MT as biomarkers of alpha—MT consumption in blood. The findings in postmortem samples were consistent with those observed in vitro, confirming the suitability of 10-donor-pooled human hepatocyte incubations as a model to predict tryptamine metabolism in humans. However, alpha—MT metabolism was different in rats in two previously published articles, due to inter-species discrepancies. Further studies on alpha—MT clinical and forensic caseworks are necessary to further understand alpha—MT metabolism.



Detecting Fentanyl Analogs by Combining Surface-Enhanced Raman Spectroscopy (SERS) and Paper Spray Mass Spectroscopy (PS-MS)

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Abstract: There is an ongoing effort in the black market to make illicit drugs more potent and addictive. Due to these continual modifications, many fentanyl analogs are developed and mixed with other illicit drugs, such as cocaine and heroin. Detecting fentanyl and fentanyl analogs in these illicit drug mixtures is a critical goal. Most confirmatory procedures require highly sophisticated laboratory equipment and long experimental procedures, which can delay critical information that might save a victim or identify a suspect. In this project, we propose miniaturizing and accelerating this process by combining surface-enhanced Raman spectroscopy (SERS) analysis and paper spray mass spectrometry (PS-MS). Combining SERS and paper-spray ionization mass spectrometry (PS-MS) would allow for quick identification of fentanyl and its analogs in complex drug mixtures. For this aim, dual-purposed paper substrates were developed by soaking them in Au/Ag nanostars. In short, we propose the combination of SERS/PS-MS by using modified paper substrates to develop rapid, portable, and reproducible methods to detect illicit drugs, especially trace amounts of fentanyl and its analogs in mixtures.





Overcoming Challenges in Analyzing THC/CBD Edibles

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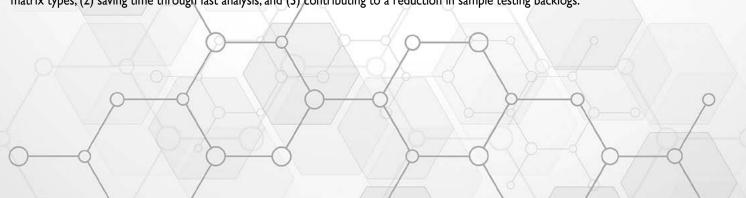
Abstract: Recreational use of Cannabis sativa, as well as the myriad of products derived from or prepared with cannabinoids, has risen exponentially with the increased legalization and decriminalization of marijuana in the U.S. Among the challenges imposed by the rise in cannabidiol (CBD)- and delta-9-tetrahydrocannabinol (Î''9-THC)-infused products is the perpetual need for highly specialized and nuanced method development to accommodate the complexity of each of the ever-changing matrices that are encountered. Current chromatography-based approaches for the detection and quantification of cannabinoids used in forensic science practice, when applied to complex materials, are generally resource-intensive, time-consuming, and require extensive sample preparation. For example, lipophilic/oily products are extracted with solvents of varying polarity, washed, dried and reconstituted. Products with high sugar and carbohydrate content, such as candies and honey, are subjected to dissolution in water, organic solvent extraction, sonication, and filtration, followed by evaporation of the solvent and derivatization. Solid foods such as brownies and cookies, are ground/homogenized prior to extraction. Aqueous products are degassed (if necessary) by sonication, and extracted with QuEChERS extraction salts. Recently, slight modifications of the recommended two-step sequence used with QueECheRS (i.e., liquid-liquid extraction and dispersive solid-phase extraction clean-up) have been employed for the extraction of cannabinoids from food products. Although many of the protocols involve routine steps, these approaches to sample analysis are often associated with the less-than-effective extraction of cannabinoids from complex matrices.

To address some of these difficulties, this study focused on the development of a more universal extraction protocol featuring the QuEChERS DisQue CEN salts that is applicable to multiple matrix types, including: (a) sweets, such as ice cream and chocolate; (d) beverages such as coffee, sodas, and liqueurs; (f) butters and oils; and (g) personal-care products such as lotions.

The approach involves suspension of the cannabinoid-containing sample in water, addition of acetonitrile followed by Waters© DisQue CEN salts, and vortexing before allowing the layers to separate. Rapid analysis of the layers by direct analysis in real time – high-resolution mass spectrometry (DART-HRMS) revealed that the cannabinoids were reliably extracted into the acetonitrile layer in a single step with recoveries of up to 99%, with no cannabinoids detected in the water/salts/matrix constituent layer.

However, the necessity of devising a means by which to differentiate between THC (scheduled) and CBD (unscheduled) is of importance to this approach: when analyzed by mass spectrometry under ambient soft ionization conditions, THC and CBD are indistinguishable because they are isomers with a molecular formula of C21H30O2 and a protonated monoisotopic mass of 315.2324. Previous findings demonstrated that derivatization using N-methyl-N-(trimethylsilyl)trifluoroacetamide (MSTFA) could reveal the presence of the two compounds within a complex matrix. Engagement of the one -OH group in THC and the two -OH groups in CBD by the derivatizing agent results in the differentiation of the two cannabinoids due to the mass disparities of the protonated adducts formed (m/z 387.2719 and 459.3114 for THC and CBD, respectively). Thus, derivatization is an important step in the process of differentiating between CBD and THC by DART-HRMS.

Overall, the development of this universal, simple, robust, and cost-effective analytical method for the extraction and quantification of cannabinoids can assist forensic science practitioners by: (1) streamlining sample analysis using a sample preparation protocol that can be applied to a vast range of matrix types; (2) saving time through fast analysis; and (3) contributing to a reduction in sample testing backlogs.





Investigating the Degradation of Benzodiazepines

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Abstract: In recent years, there has been a significant increase in the number of novel psychoactive substances (NPS) encountered by crime laboratories, including designer benzodiazepines. As an example, in 2022 the Houston Forensic Science Center (HFSC) detected eleven different benzodiazepines in seized drug evidence, eight of which were designer NPS. These drugs are frequently used in drug-facilitated crimes, such as robberies and sexual assaults. It is therefore essential to develop tools that can rapidly and reliably screen for these compounds, as well as their traditional benzodiazepine counterparts. The aim of this study is to investigate the effect of pH on the stability of selected benzodiazepine compounds, to identify degradation products observed using UV-Vis spectrophotometry and gas chromatography-mass spectrometry (GC-MS) and to provide a more comprehensive understanding of the UV-Vis data obtained after exposure of these compounds to ultraviolet light under strong acidic conditions.

The benzodiazepines analyzed in this study were selected with the aid of the HFSC based on compounds commonly encountered in their current casework and included traditional benzodiazepines, such as alprazolam and diazepam, and designer benzodiazepines, such as flubromazepam, 4'-chloro deschloroalprazolam, and bromazolam. These compounds were prepared in 2/3 N sulfuric acid (H2SO4) and analyzed using a UV-Vis spectrophotometer to assess the linearity of the method. Serial dilutions of each benzodiazepine analyzed in this study were performed in 2/3 N H2SO4 at concentrations of 20, 16, 12, 8, 4, 2, 1.6, 1.2, 0.80, 0.40, and 0.20 ppm to determine their linearity. All compounds, aside from phenazolam, phenazepam, clonazepam, and flunitrazepam, exhibited good linearity with coefficient of determination values (R2 values) above 0.99. The benzodiazepines with lower R2 values correlated with weak absorption in the UV region compared to the benzodiazepines with higher R2 values. Solutions were also prepared for selected traditional (e.g., alprazolam and diazepam) and designer benzodiazepines (e.g., 4'-chlorodeschloroalprazolam and flubromazepam) in phosphate buffer, methanol, and sodium hydroxide to evaluate the effects of varying pH on benzodiazepine stabilities. Absorbance spectral data was acquired from the benzodiazepines using a UV-Vis spectrophotometer with a wavelength range of 220-340 nm. Initial work conducted by the HFSC showed UV-Vis spectra exhibiting a shift in lambda max when comparing the initial scan and subsequent scans following approximately 10 minutes of UV exposure for several traditional and designer benzodiazepines, such as alprazolam, bromazolam, and 4'-chloro deschloroalprazolam. When replicating this data at Sam Houston State University (SHSU), however, the spectra obtained only showed the post-UV exposure lambda max. For example, analyzing alprazolam immediately after being dissolved in 2/3 N H2SO4 resulted in a broad absorption band in the 250-280 nm region with a lambda max at approximately 278 nm. However, when analysis of alprazolam was delayed, the spectrum showed a shift in lambda max to approximately 260 nm. Based on this observation, it can be inferred that the shift in the UV spectra may be attributed to the samples' interaction with the acid solution before its analysis, which indicates that the pH effect of the strong acid may be more influential on the stability of the compound than exposure to UV light.

Next steps in this research include examining the effect of varying pH conditions by collecting the UV-Vis spectra for traditional benzodiazepines, alprazolam and diazepam, and designer benzodiazepines, 43€TM-chloro deschloroalprazolam and flubromazepam. UV-Vis spectra have been collected for each compound in methanol, and data collection in phosphate buffer and sodium hydroxide solutions is in progress. Previous studies have shown diazepam to be highly stable at neutral pH whereas alprazolam is least stable at neutral pH conditions. Previous literature also indicated certain benzodiazepines to be more stable in neutral pH whereas others prefer a more basic or acidic environment. The compounds showing shifts in their UV-Vis spectra in the different solutions will be extracted and GC-MS analysis will be carried out to identify degradation products. Differences in the degradation products identified in the different pH solutions will also be examined to determine how pH influences their formation.



Profiling Tablets For Unknown Compounds Using HDX-HRMS

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Abstract: The number of emerging psychoactive compounds is constantly increasing. However, mass spectral libraries based on LC-MS or GC-MS cannot be updated as quickly and not all putative reference substances can be purchased, so other strategies have to be applied.

We investigated the principle of HDX (hydrogen deuterium exchange) combined with HR-MS/MS (high-resolution mass spectrometry) by analyzing a blue tablet with Punisher embossing from a forensic case study. Our screening study revealed that the tablet contained MDMA and two previously unknown compounds (UC#I and UC#2) which eluted after MDMA. As proof of concept, we dissolved an aliquot of the tablet in deuterium oxide/acetonitrile and diluted the solution to 100 ng/ml with deuterium oxide. In parallel, we dissolved another aliquot of the tablet in water/acetonitrile and diluted it with water. Finally, we analyzed both solutions with our SCIEX X500R QToF mass spectrometer by direct injection to obtain the [M+D]+ and [M+H]+ adduct and thus the number of exchangeable protons.

We monitored one exchangeable proton for MDMA ([M+H]+: 204.137 and [M+D]+: 205.145), two for UC#1 ([M+H]+: 248.127 and [M+D]+: 250.141) and three for UC#2 ([M+H]+: 329.221 and [M+D]+: 332.24). Next, we fragmented the exchanged [M+D]+ and non-exchanged [M+H]+ quasi-molecular ions at 10 eV, 25 eV and 35 eV, whereupon the MS/MS spectrum at 25 eV appeared to be the most informative due to the presence of the quasi-molecular ion and abundant fragment ions. We then compared the two CID-MS spectra. For compound UC#1 we observed a similar MS/MS spectrum for both quasi molecular ions except for the fragment at m/z 122.059. Here the MS/MS spectrum of the [M+D]+ ion showed a peak at m/z 123.063. For UC#2 we observed fragment mass shifts for m/z 166.049 (C8H8NO3+), m/z 123.044 (C7H7O2+) and m/z 105.034 (C7H5O+). Finally, we identified UC#1 as N-cyclohexylbenzamide and UC#2 as carboxy-N-cyclohexylbenzamide. These are most probably impurities whose harmful effect on the organism still needs to be clarified.

This study shows that HDX-HRMS is a powerful approach for characterizing unknown compounds. Although this method is only a small piece of puzzle in the structure elucidation of unknown compounds, it can at least be used to identify chemical substance classes. If the laboratory is well equipped, the liquid chromatograph can be placed under deuterium oxide, allowing more complex samples to be analyzed.





Evaluation of Sample Ionization Sources for the Characterization of Isomeric Fentanyl Analogs Utilizing Trapped Ion Mobility Spectrometry Time of Flight Mass Spectrometry (TIMS-ToF MS).

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Abstract:

Introduction

Worldwide, especially in the United States, the public has been increasingly impacted by the utilization of fentanyl and the rise of its analogs in the early 2010s. Ever since, fentanyl has risen to become one of the leading causes of drug-related deaths in the United States. In recent years, it has consistently ranked among the top substances involved in fatal overdoses and fentanyl-related fatalities have surpassed deaths caused by other opioids, such as prescription painkillers and heroin.

This study aims to assess the utilization of various sample introduction ionization sources (direct infusion electrospray (ESI), nanoESI, direct analysis in real time (DART) coupled with trapped ion mobility spectrometry (TIMS) and mass spectrometry (MS). Employing these orthogonal techniques to comprehensively characterize fentanyl analogs by thoroughly investigating their isotopic distributions, characteristic ion mobility profiles, and fragmentation patterns.

Methods

A Fentanyl Analog Screening Kit was acquired from Cayman Chemicals, which contained over 200 synthetic opioids. Standards were prepared in methanol and diluted to a concentration of I ng/mL (I ppb). Isomeric standards were organized into separate sample sets for their initial characterization. Experiments were performed on a custom built TIMS-q-ToF MS (Bruker Daltonics) equipped with a custom nESI, DART ionization source, or coupled to a Shimadzu Prominence HPLC (Shimadzu) for direct infusion experiments equipped with an Phenomenex Onyx monolithic C18 column (100 x 4.6 mm) from prior to ion mobility and MS analysis. Initial experiments were performed in positive ion mode using data dependent acquisition and data independent acquisition with resulting data processed using Data Analysis 5.2 software (Bruker Daltonics).

Preliminary Data

29 isomeric sets totaling 185 fentanyl analogs were characterized by examination of the 2D LC-MS and IMS-MS profiles which allowed for the identification based on their resulting isotopic pattern, retention time (direct infusion) and/or ion mobility profiles (with many previously unreported). Characteristic MS/MS spectra were collected for all fentanyl standards and resulting data indicated that most isomers can be separated via LC (retention times, RT). In other experiments, where analyte separation could not be achieved via RT, analytes were able to be separated in the ion mobility domain. All ionization sources produced analyte species were observed in their protonated form [M+H]I+. A trend was observed where analytes produced a single chromatographic peak but often displayed two ion mobility bands likely do to differing protonation schemes. TIMS spectra showed a typical resolving power of around 100. Inspection of the MS/MS profiles showed similarities across the isomers, highlighting the need for chromatographic or ion mobility separation. Current experiments are focused on the determination of the ionization efficiency, LOD, and reproducibility of the orthogonal ionization sources.



From Sample to Results in Seconds: DART Ionization with Trapped Ion Mobility QTOF MS for Fast Identification of Seized Drugs

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Abstract:

Background and aim:

Forensic analytics are constantly facing growing demands including an increasing number of targets due to emerging new psychoactive substances and the need to shorten response time and increase throughput. The use of Direct Analysis in Real Time with High Resolution Mass Spectrometry (DART-HRMS) as a forensic tool has been praised for its ability to quickly and easily generate valuable information. Herein, we present a workflow based on the combination of DART-HRMS with trapped ion mobility spectrometry (TIMS) for the identification of seized drugs including isomeric substances.

Methods:

A DART JumpShot source (Bruker Daltonics) and a timsTOF Pro 2 mass spectrometer (Bruker Daltonics) were used for the analysis. 3 µL aliquots of sample solutions containing mixtures of different drugs including opioids, benzodiazepines, amphetamines etc. and isomeric substance pairs were deposited onto QuickStrip wire mesh grid cards. Alternatively, a very small amount of drug powder could be deposited on a glass stick and ionized from there without any additional sample preparation. The DART source was operated with helium in pulsed gas flow ionization mode at a temperature of 350° C. Full scan and parallel accumulation serial fragmentation (PASEF) MS/MS spectra were acquired in positive ionization mode and searched against home-built libraries containing about 250 drugs and toxins as well as 3rd party libraries, e.g. from NIST.

Results:

Up to 20 different drugs could be separated and identified in one sample. Using TIMS, pairs of isomeric substances including morphine and norcodeine as well as hydromorphone and norhydrocodone could be separated, yielding clean MS/MS spectra for library searches. Collision cross-sections (CCS) were used as an additional identification criterion to assist in the identification of the drugs. Together with Bruker's automated library search for DART-MS/MS data, sample reports were received in less than 15 s after sample introduction.

Conclusion:

The proposed workflow provides a comprehensive solution for the characterization of seized drugs. Compared to analysis times of several minutes with chromatographic methods, analyses with DART-MS are completed within 15 seconds. Ion mobility can be used to clean up spectra and improve identification certainty. Additionally, little to no sample preparation is required.

Keywords: DART, seized drugs, trapped ion mobility spectrometry

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Sabra R. Jones, PhD, D-ABFT-FT Regional Toxicology Liaison, NHTSA Region 5 **Scientific Program Chair**

Sabra Jones is a board-certified Forensic Toxicologist with a focus on transportation safety. Sabra is the Regional Toxicology Liaison for the National Highway Traffic Safety Administration's Region 5, serving Illinois, Indiana, Michigan, Minnesota, Ohio, and Wisconsin. Sabra has worked in transportation safety at the Federal Aviation Administration and driving impairment, in addition to other areas of forensic toxicology at the Tarrant County Medical Examiner's office. She served as an Assistant Professor and graduate student mentor at Boston University School of Medicine's Biomedical Forensic Sciences program. She conducts research in the areas of forensic toxicology,

analytical chemistry, and impairment.

Sabra earned her Master of Science degrees in Drug Chemistry and Forensic Toxicology from the University of Florida as well as undergraduate and graduate degrees in Criminal Justice from the University of Central Oklahoma. Sabra received her Ph.D. from Oklahoma State University, Center for Health Science in Forensic Science.

She serves as the immediate past Chair and on the Executive Board of the National Safety Council's Alcohol, Drugs, and Impairment Division. She serves as Vice Chair of the Academy Standards Board's Toxicology Consensus Body. Sabra is active in several professional organizations such as the Society of Forensic Toxicologists, Northeastern Association of Forensic Scientists, and the American Academy of Forensic Sciences where she has served as the chair of the toxicology section. Sabra was appointed by the Commonwealth of Massachusetts's Governor Charles Baker to serve on the Forensic Oversight Board and the Special Commission on Operating Under the Influence and Impaired Driving.

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Dr Lorna A. Nisbet Scientific Co-Chair

Lorna Nisbet is currently a Senior Lecturer and Principal Investigator in Forensic Toxicology at the Leverhulme research Centre for Forensic Science, University of Dundee. She obtained her BSc (Hons) in Analytical Chemistry from the University of Strathclyde, Glasgow, before completing her MSc in Forensic Toxicology at the University of Glasgow. Lorna then went on to obtain her PhD in Forensic Toxicology at the University of Glasgow focusing on the detection of new psychoactive substances in biological matrices. As part of her PhD Lorna spent 15 months carrying out research at the Fredric Rieder's Family Renaissance Foundation in Philadelphia, USA.

Lorna is also a member of the Royal Society of Chemistry, the American Academy of Forensic Science, the Society of Forensic Toxicologists, the United Kingdom and Ireland Association of Forensic Toxicologists, the LTG and the European Workplace Drug Testing Society.

