

KBC at Umeå University and SLU Umeå, Sweden

Current Trends in Applied Mass Spectrometry 2025

Conference Program and Abstracts

Theresa Kieselbach
2025-04-04

Table of Content

Current Trends in Applied Mass Spectrometry	3
Abstract	3
Abbreviations	4
Acknowledgements	5
Organizers	5
Contact	5
Funding	6
Sponsors and funders	6
Companies	6
Infrastructures	6
Organizations	6
Program of the workshops on 19 March 2025	7
09:00 – 10:30 <i>Workshop by Agilent</i>	7
10:30 – 12:00 Workshop av Teknolab Sorbent AB and Extraction Technologies Norway AS.....	7
12:00 – 13:00 Lunch.....	7
13:00 – 16:00 Workshop by SMC and Umeå University Library in collaboration with EMBL-EBI	7
Program of the conference and fair on 20 March 2025	8
9:00 The reception desk opens in the KBC Hall.	8
10:15 – 16:30 Conference in the Carl-Kempe Hall (KBE303) and fair in KBC Glasburen and the KBC Hall.	8
10:15 – 10:20 Jonas Bergquist, SMSS. Welcome speech.	8
10:20 – 10:55 Anders Feldthus and Deepak Luthra, Agilent. PFAS analysis by GC-MS and LC-MSMS. Accurate quantification at trace level in different matrices.	8
10:55 – 11:30 Noud van der Borg, Bruker Netherlands. Fast screening and quantification of seized drugs.	8
11:30 – 12:05 Ross Chawner, Waters Corporation. Rapid Data Rationalization for Biotransformation using the Xevo MRT Mass Spectrometer with Dedicated Data-Mining Software.....	8
12:05 – 13:35 Lunch break and opportunity to visit the fair and to talk to the representatives of the companies.	8
13:35 – 14:10 Tony Wiklund, Thermo Fisher Scientific Sweden. Thermo Fisher innovation - How can you bridge the gap between discovery and the clinic?	8
14.10 – 14:45 Magnus Olin, Shimadzu Sweden. OAD – Oxygen attachment dissociation – A novel, unique, selective MS/MS fragmentation technology that specifically fragments at a C=C bond position.	8

Current Trends in Applied Mass Spectrometry at the KBC Umeå on 19 and 20 March 2025

14:45 – 15:15	Coffee break and opportunity to visit the fair and to talk to the representatives of the companies.	8
15:15 – 15:50	Anders Dahl Knudsen, Sciex. SCIEX Advances in Mass Spectrometry for Metabolomics – 7500+, ZenoTOF and EAD fragmentation.....	8
15:50 – 16:25	Linus Svenberg, LECO Nordic AB. Non-Targeted Analysis using comprehensive-two-dimensional gas chromatography coupled to a mass spectrometry.....	8
16:25 – 16:30	Theresa Kieselbach (SMSS) and Annika Johansson (SMC). Closing speech.	8
Dinner after the event.....		8
Workshop abstracts		9
Agilent MassHunter, your trusted answer for analyte identification and quantification.....		9
Electromembrane Extraction (EME) – New technology for green efficient and highly selective sample preparation of biological samples		10
How the MetaboLights repository can help you to put Open Science into practice in metabolomics research.....		12
Conference abstracts		13
PFAS analysis by GC-MS and LC-MSMS. Accurate quantification at trace level in different matrices		13
Fast Screening and Quantification of Seized Drugs		14
Rapid Data Rationalization for Biotransformation using the Xevo MRT Mass Spectrometer with Dedicated Data-Mining Software		15
Thermo Fisher innovation - How can you bridge the gap between discovery and the clinic?17		
OAD – Oxygen attachment dissociation – A novel, unique, selective MS/MS fragmentation technology that specifically fragments at a C=C bond position.....		18
SCIEX Advances in Mass Spectrometry for Metabolomics – 7500+, ZenoTOF and EAD fragmentation		19
Non-Targeted Analysis using comprehensive-two-dimensional gas chromatography coupled to a mass spectrometry.....		21
Companies represented at the fair.....		22
Agilent		22
Bruker		22
Hamilton Nordic.....		22
LECO		23
Sciex.....		23
Shimadzu.....		23
Teknolab Sorbent AB and Extraction Technologies Norway AS (ETN)		23
Thermo Fisher Scientific		24
Waters		24
Author of this booklet.....		24

Current Trends in Applied Mass Spectrometry

Abstract

This booklet contains the program and the abstracts of the presentations and the workshops of the conference Current Trends in Applied Mass Spectrometry on March 19th and 20th, 2025 at the KBC at Umeå University and SLU Umeå. It also gives an account of the organizers, the contributing organizations and companies, and the funding of this conference.

This conference is a forum for representatives of industry, infrastructures and researchers in academia to meet one another and to discuss the latest innovations in the field of applied mass spectrometry and possible solutions to analytical problems. It consists of a day with workshops on March 19th, 2025, and a day with a conference and a fair on March 20th, 2025.

The workshops cover selected topics of the workflow of applied mass spectrometry and of the communication of the scientific results. They include an introduction to the Mass Hunter software by Agilent and to sample purification through the electromembrane extraction technology by ETN. In addition, EMBL-EBI, the Swedish Metabolomics Centre (SMC), and Umeå University Library give a hands-on workshop about Open Science and how the MetaboLights repository can help researchers in metabolomics to put it into practice.

The conference presentations highlight latest achievements in the technology of LC-MSMS and GC-MS to resolve challenging problems in the identification, structural analysis and quantification of small molecules. Agilent discusses challenges and advancements in the accurate quantification of multiple PFAS compounds at trace levels. Bruker introduces Direct Analysis in Real Time with High Resolution Mass Spectrometry (DART-HRMS) that allows rapid detection and structural analysis of drugs, pesticides and other compound classes in a chromatography-free workflow. Waters presents a novel data-independent and data dependent workflow for metabolite characterization in biotransformation studies using high resolution mass spectrometry.

Thermo Fisher Scientific presents the novel Stellar™ MS technology and its capabilities for a fast and sensitive targeted quantification of compounds and the opportunities that it offers in a transition from discovery to clinical practice. Shimadzu introduces and discusses the opportunities of the Oxygen Attachment Dissociation (OAD) technology that specifically breaks C=C bonds and the advantages that it provides for the analysis of lipids.

Sciex introduces the advantages of electron activated dissociation (EAD) fragmentation and ZenoTOF technology to create high quality MS2 spectra that allow, for instance, the structural analysis of unknown metabolites and the quantification of lipid isomers. LECO presents an application of two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GCxGC-TOFMS) to achieve enhanced separation of compounds and high-speed acquisition across the full mass range. In this application, a novel Multi-Mode Source (MMS) was used that can perform EI/CI ionization. This technology provides library-searchable spectra with accurate masses for improved confidence of identification.

In summary, this conference offers of a unique opportunity to learn about the latest innovations in Applied Mass Spectrometry and to discuss analytical problems with experts in the field. In addition, it connects Applied Mass Spectrometry and Open Science and offers researchers in metabolomics an opportunity to learn how one can design holistic workflows that can resolve challenging analytical problems and ensure timely scholarly communication.

Abbreviations

DART-HRMS: Direct analysis in real time with high resolution mass spectrometry

EAD: Electron activated dissociation

EI/CI: Electron impact ionization and chemical ionization

EMBL: European Molecular Biology Laboratory

EMBL-EBI: EMBL's European Bioinformatics Institute

ETN: Extraction Technologies Norway AS

GC-MS: Gas chromatography couples to mass spectrometry

GCxGC-TOFMS: two-dimensional gas chromatography separation coupled to tandem mass spectrometry

KBC: Chemical Biological Centre (Kemiskt biologiskt centrum) at Umeå University

LC-MSMS: Liquid chromatography coupled to tandem mass spectrometry

MMS: Multi mode (ion) source

MS: Mass spectrometry

MS2: Tandem mass spectrometry that creates fragment mass spectra derived from an unfragmented mother ion

OAD: Oxygen attachment dissociation

PFAS: Per- and polyfluoroalkyl substances

SLU: Sveriges lantbruksuniversitet (Swedish University of Agricultural Sciences)

SMC: Swedish Metabolomics Centre

SMSS: Swedish Mass Spectrometry Society

ZenoTOF technology: Zeno trap time of flight (mass spectrometry) technology

Acknowledgements

The organizers thank the participating companies and their representatives because they make this conference possible by contributing to it with funding, presentations and workshops. In addition, the organizers thank Umeå University for a conference grant.

The organizers also thank Victoria Yan from EMBL Open Science and Noemi Tejera, Thomas Payne and Ozgur Yurekten from EMBL EBI for their kind and invaluable help to prepare and to teach the workshop on Open Science and the MetaboLights repository.

Furthermore, the organizers thank Anna Shevtsova and Rebecca Forsberg at the KBC Communication Office for setting up the event home page and for their very useful professional advice to organize the logistics of the conference. Added to this the support by the SMSS board and by SciLifeLab is greatly appreciated.

2025-04-04/Theresa Kieselbach and Annika Johansson

Organizers

The organizers of this event are the SMSS (Swedish Mass Spectrometry Society) and the SMC (Swedish Metabolomics Centre) at the KBC Umeå in collaboration with the Mass Spectrometry Network Umeå. In addition, EMBL-EBI and Umeå University Library are involved in the preparation and the teaching of the workshop on Open Science and the MetaboLights repository.

Contact

Theresa Kieselbach, email: theresa.kieselbach@umu.se

Theresa serves on the board of the SMSS (Swedish Mass Spectrometry Society) as representative for Umeå and is a research coordinator at Umeå University Library. The SMSS is a division of the Swedish Chemical Society (Kemisamfundet).

Funding

The conference and the workshops are non-profit events that are organized on a self-cost basis. The funding came from a conference grant from Umeå University (dnr: FS 2.1.6-2005-24), from the Swedish Metabolomics Centre and from the companies who presented their innovations at this conference. The conference grant and the sponsor contributions covered the costs for food, room rent, and name badges. Travel costs were not part of the conference budget, and everybody paid for their trip to attend the conference and its workshops.

Sponsors and funders

Companies

- Agilent
- Bruker
- Hamilton Nordic AB
- LECO
- Sciex
- Shimadzu
- Teknolab Sorbet AB and Extraction Technologies Norway AS
- Thermo Fisher Scientific
- Waters

Infrastructures

- Swedish Metabolomics Centre

Organizations

- Umeå University

Program of the workshops on 19 March 2025

09:00 – 10:30 *Workshop by Agilent*

Title: Agilent MassHunter, your trusted answer for analyte identification and quantification

Instructor: James Waddington, PhD, LC-MS Application Engineer, Agilent, UK

Location: small lecture hall at the KBC (KBE301) ([View the small lecture hall on the digital campus map.](#))

10:30 – 12:00 *Workshop av Teknolab Sorbent AB and Extraction Technologies Norway AS*

Title: Electromembrane Extraction - Gold standard in sample preparation

Instructor: Professor Stig Pedersen-Bjergaard - Section for Pharmaceutical Chemistry at University of Oslo, Norway

Location: Stora fokusrummet ([View Stora fokusrummet on the digital campus map.](#))

12:00 – 13:00 *Lunch*

The organizers do not provide lunch.

13:00 – 16:00 *Workshop by SMC and Umeå University Library in collaboration with EMBL-EBI*

Title: How the MetaboLights repository can help you to put Open Science into practice in metabolomics research

Instructors:

Noemi Tejera Hernandez, European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, Cambridge CB10 1SD, UK

Ozgur Yurekten, European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, Cambridge CB10 1SD, UK

Annika Johansson, Swedish Metabolomics Centre, Department of Plant Physiology, Umeå University, 90187 Umeå, Sweden

Theresa Kieselbach, Umeå University Library, Umeå University, 90187 Sweden

Location: Stora fokusrummet ([View Stora fokusrummet on the digital campus map.](#))

Note: Noemi Tejera and Ozgur Yurekten will give this workshop on-line and Annika Johansson and Theresa Kieselbach will be instructors on-site.

Program of the conference and fair on 20 March 2025

- 9:00 The reception desk opens in the KBC Hall.
([View the KBC on the digital campus map.](#))
- 10:15 – 16:30 Conference in the Carl-Kempe Hall (KBE303) and fair in KBC Glasburen and the KBC Hall.
([View the Carl-Kempe Hall on the digital campus map.](#) [View KBC Glasburen on the digital campus map.](#))
- 10:15 – 10:20 Jonas Bergquist, SMSS. Welcome speech.
- 10:20 – 10:55 Anders Feldthus and Deepak Luthra, Agilent. PFAS analysis by GC-MS and LC-MSMS. Accurate quantification at trace level in different matrices.
- 10:55 – 11:30 Noud van der Borg, Bruker Netherlands. Fast screening and quantification of seized drugs.
- 11:30 – 12:05 Ross Chawner, Waters Corporation. Rapid Data Rationalization for Biotransformation using the Xevo MRT Mass Spectrometer with Dedicated Data-Mining Software.
- 12:05 – 13:35 Lunch break and opportunity to visit the fair and to talk to the representatives of the companies.
- 13:35 – 14:10 Tony Wiklund, Thermo Fisher Scientific Sweden. Thermo Fisher innovation - How can you bridge the gap between discovery and the clinic?
- 14:10 – 14:45 Magnus Olin, Shimadzu Sweden. OAD – Oxygen attachment dissociation – A novel, unique, selective MS/MS fragmentation technology that specifically fragments at a C=C bond position.
- 14:45 – 15:15 Coffee break and opportunity to visit the fair and to talk to the representatives of the companies.
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- 15:50 – 16:25 Linus Svenberg, LECO Nordic AB. Non-Targeted Analysis using comprehensive-two-dimensional gas chromatography coupled to a mass spectrometry.
- 16:25 – 16:30 Theresa Kieselbach, SMSS. Closing speech.

Dinner after the event

You are welcome to come to a dinner at a restaurant after the meeting. The costs for this dinner are not covered by the conference and you must pay for them privately. The organizers will share details about time and location at the conference.

Workshop abstracts

Agilent MassHunter, your trusted answer for analyte identification and quantification

James Waddington, PhD, LC-MS Application Engineer, Agilent, UK

Tired of the unknown? In this expert led workshop we will showcase how the Agilent MassHunter software suite can simplify your day-to-day lab operation and data analysis, leaving you time to focus on other things in the lab that matter. We will cover a range of topics, focussed on Life Science research, from data acquisition to statistical analysis. Throughout the interactive session we will aim to cover a range of applications, sharing hints and tips on how to get the best data possible from your samples. Whether you're interested in metabolites, lipids, peptides or proteins, we've got a solution for you.

The workshop will be focussed on the analysis of high-resolution accurate mass (HRAM) data from our range of LC-QTOF instrumentation. Automated workflows to turn your spectra into compounds will be shown, with the help of our powerful library management software ChemVista. We know that identification is often only one part of the story, with quantification a key component of any experiment. Quantitative analysis tailored to you will be demonstrated, with streamlined approaches to speed up your analysis described. Finally, user-friendly downstream statistical data analysis will also be explored using our latest addition to the suite, MassHunter Explorer.

We invite scientists and technicians from all levels of expertise to join us. Better yet, our Application Specialist will be on hand to answer any specific questions you have throughout the day.

References for further reading

MassHunter Masterclass Webinar Series: <https://lnkd.in/dH5wrWR3>

MassHunter software suite: <https://www.agilent.com/cs/library/brochures/brochure-masshunter-software-5994-4923en-agilent.pdf>

MassHunter Explorer: <https://www.agilent.com/cs/library/brochures/masshunter-explorer-5994-6107en-agilent.pdf>

ChemVista: <https://www.agilent.com/cs/library/brochures/br-chemvista-software-5994-5965en-agilent.pdf>

Electromembrane Extraction (EME) – New technology for green efficient and highly selective sample preparation of biological samples

Stig Pedersen-Bjergaard, Section for Pharmaceutical Chemistry, University of Oslo, Norway

This course offers a comprehensive introduction to electromembrane extraction (EME), a recently commercialized and innovative addition to the analytical chemistry toolbox. EME is a microextraction technique applicable for acids, bases, and permanently ionic compounds. It involves the extraction of target analytes from an aqueous sample, across a liquid membrane, and into an acceptor solution, all facilitated by an external electrical field. The liquid membrane consists of a few microliters of organic solvent immobilized within the pores of a filter membrane, while the acceptor solution is a microliter volume of pure aqueous buffer.

EME stands out for its unique selectivity, which can be fine-tuned by adjusting the direction and magnitude of the electrical field, the chemical composition of the liquid membrane, and pH. As a green approach to sample preparation, EME minimizes the use of solvents and chemicals. It provides efficient cleanup of complex samples such as blood, and the aqueous acceptor solutions can be directly injected into LC/LC-MS systems without further processing.

This course will focus on introducing the fundamental principles of EME, covering method development, applications, advantages, and limitations, as well as its potential as a cutting-edge sample preparation technique. It is ideal for those interested in eco-friendly sample preparation methods and pioneering research into emerging concepts and technologies. With the growing importance of green sample preparation and the availability of commercial equipment, EME offers a sustainable alternative for scientists. Innovative research related to EME is expected to increase in the future, due to the unique flexibility of the concept. Understanding the basics of EME, as given in this short course, is a major advantage both in the green and innovative direction.

In this workshop you will get to know:

- The EME principle
- How to develop an EME method

Be the first in Sweden to get knowledge and experience about EME.

References for further reading

ETN, Electromembrane extraction (EME) vs. SPE and LLE. 2024 Oct 7. https://cdn.prod.website-files.com/5eb27d32b7f1ceff62ec3965/671fba7910f66ec199875276_EME%20vs%20SPE%20and%20LLE.pdf

Oldeide Hay A, Trones R, Herfindal L, Skrede S, Hansen FA. Determination of methotrexate and its metabolites in human plasma by electromembrane extraction in conductive vials followed by LC-MS/MS. *Advances in Sample Preparation*, 2: 100011. <https://doi.org/10.1016/j.sampre.2022.100011>.

Schüller M, Bergh MS, Pedersen-Bjergaard S, Øiestad EL. Electromembrane extraction of drugs of abuse and prescription drugs from micropulverized hair. *J Anal Toxicol.* 2024 Aug 21;48(7):489-498. doi: 10.1093/jat/bkae051. PMID: 38905017; PMCID: PMC11336399.

Skaalvik TG, Øiestad EL, Pedersen-Bjergaard S, Hegstad S. Determination of amphetamine enantiomers in urine by conductive vial electromembrane extraction and ultra-high performance supercritical fluid chromatography tandem mass spectrometry. *Drug Test Anal.* 2023 Aug;15(8):909-918. doi: 10.1002/dta.3487. Epub 2023 May 10. PMID: 37114617.

Please check also out the ETN webpage about how to do EME at: <https://how-to-eme.com/>

If you interested in more publications about EME, please also have a look at our list of selected publications on our home page at: <https://www.etn-eme.com/publications>

Contact

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How the MetaboLights repository can help you to put Open Science into practice in metabolomics research

Noemi Tejera ¹⁾, Ozgur Yurekten¹⁾, Annika Johansson^{2) 3)} and Theresa Kieselbach⁴⁾

- 1) *European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, Cambridge CB10 1SD, UK*
- 2) *Department of Plant Physiology, Umeå University, 90187 Umeå, Sweden*
- 3) *Swedish Metabolomics Centre, Department of Plant Physiology, Umeå University, 90187 Umeå, Sweden*
- 4) *Umeå University Library, Umeå University, 90187 Sweden*

This workshop will give you an introduction to Open Science policies that are relevant for your research work and to the FAIR-data principles. You will also learn how you can take advantage of the MetaboLights repository at EMBL-EBI to put Open Science into practice and create a citable research output, if you do research in metabolomics. The workshop consists of three parts that include:

1. Introduction to Open Science and Open Science policies
2. Introduction to MetaboLights
3. Hands-on session on how to create a submission to MetaboLights. Data standards and essential requirements to create a citable research output using experimental data and metadata from metabolomics experiments in this database.

This workshop complements to the workshop [Metabolomics in Molecular Medicine in the autumn of 2024](#), and it is relevant for everybody who wants to give access to research data from metabolomics experiments to meet Open Science requirements by a funder, a journal, or a research organization. It covers the necessary theory and includes a hands-on part to learn how to prepare data and metadata from metabolomics experiments for submission to MetaboLights. It does not matter if you already have data from existing metabolomics experiments or if you are going to create such data in your future research. In either case this workshop will give you help to get started and to proceed on your own.

References for further reading

Swedish University of Agricultural Sciences. (2022). Policy on the management of and open access to research and environmental monitoring and assessment data at SLU. URL: <https://www.slu.se/en/subweb/library/publish-and-analyse/archiving-and-publishing-research-data/slus-datahanteringspolicy/>

Umeå University. (2021). Research data policy. Reg. no.: FS 1.1.-545-21. URL: Reg. no.: FS 1.1.-545-21. URL: <https://www.umu.se/en/legal-framework/research/research-data-policy/>

Yurekten, O., Payne, T., Tejera, N., Amaladoss, F. X., Martin, C., Williams, M., & O'Donovan, C. (2024). MetaboLights: open data repository for metabolomics. *Nucleic acids research*, 52(D1), D640–D646. <https://doi.org/10.1093/nar/gkad1045>

MetaboLights online tutorial 'Quick tour'. URL: <https://www.ebi.ac.uk/training/online/courses/metabolights-quick-tour/>.
<https://doi.org/10.6019/TOL.MbL-qt.2012.00001.1>

Contact

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Conference abstracts

PFAS analysis by GC-MS and LC-MSMS. Accurate quantification at trace level in different matrices

Anders Feldthus and Deepak Luthra, Agilent

PFAS also known as forever chemicals, was the magical wonders of science with usage from Textile to Pans. These chemicals entered in our food chain, environment and even in blood. Highly sensitive Mass Spec are the need of time to detect traces of these chemicals in matrices like Air, Water, Food with advanced sample prep techniques and sample introduction devices to handle difficult matrices like Air and blood. We present comprehensive analysis of PFAS in various matrices using Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS) system and GCMS. The methodology involves optimized sample preparation techniques tailored for different matrices, including water, soil, and biological samples. The Agilent LC-MS/MS system's high sensitivity and specificity enable the accurate quantification of multiple PFAS compounds at trace levels. Results demonstrate the system's robustness and reliability in detecting PFAS across diverse environmental and biological samples, highlighting its potential for widespread application in environmental monitoring and public health studies. This presentation will discuss the analytical challenges, methodological advancements, and implications of PFAS detection in different matrices.

References for further reading

Damen, C., Kornas, P., van der Molen, R. (2024). Quantitation of Per- and Polyfluoroalkyl Substances (PFAS) in Chicken Eggs for Human Consumption. Agilent Technologies Inc. Application Note 5994-7358EN. URL: <https://www.agilent.com/cs/library/applications/an-pfas-eggs-consumption-bond-elut-carbons-5994-7358en-agilent.pdf>

Zhao, L., Giardina, M., Parry, E. (2024). Determination of 30 Per- and Polyfluoroalkyl Substances in Beef, Tuna, and Shrimp. Agilent Technologies Inc. Application Note 5994-7368EN. URL: <https://www.agilent.com/cs/library/applications/an-pfas-captiva-emr-food-5994-7368en-agilent.pdf>

Zhou, A. (2024). PFAS Quantitation from Food Contact Materials Using the Agilent 6495D Triple Quadrupole LC/MS System. Agilent Technologies Inc. 5994-7889EN.

If you would like to have a PDF copy of the application note by Zhou (2024), please contact Arash Aria.

Contact

Anders Feldthus, Agilent, email: anders.feldthus@agilent.com

Arash Aria, Agilent, email: arash.aria@agilent.com

Fast Screening and Quantification of Seized Drugs

Noud van der Borg, Bruker Daltonics

Since many years Mass Spectrometry is moving into many laboratories. Just two decades ago, having a MS system in your lab was an exception, due to cost and complexity. Nowadays many applications moved from UV, Electrochemical or fluorescence detector to GC-MS or LC-MS. The number of samples continues growing. Particularly solvent costs are permanently increasing. Faster and green (pre)screening is a real trend in analysis. Seized Drugs analysis as well as some specific Food and Environmental applications are already investigated or even developed. This talk will give an update on the status of this rapid and fast-expanding analytical workflow and introduce Direct Analysis in Real Time with High Resolution Mass Spectrometry (DART-HRMS). DART-HRMS allows rapid detection and structural analysis of drugs, pesticides and other compound classes in a chromatography-free workflow. Although the MS method is almost the same in different applications, the sample preparation will depend on matrix, required sensitivity and needed selectivity. Seconds instead of minutes analysis time will bring the next revolution into your lab.

References for further reading

Lopez, J. (2024). EVOQ® DART-TQ+ enables fast, sensitive pesticide analysis in food. Bruker Applied Mass Spectrometry. AMS-018 1912150. URL: https://www.bruker.com/en/landingpages/bams/markets/food-beverage/_jcr_content/root/sections/section_1354282499_c/sectionpar/standardteaser_copy/it-ems/standardteaseritem_c.download-asset.pdf/link/1912150-ams-018-enabling-fast-and-sensitive-pesticide-analysis-in-food-ebook.pdf

Niehaus, E.-M., Baessmann, C., Groeschel, L., Nordhorn, I. (2024). A new paradigm in forensic analysis. DART-MS enables the rapid chromatography-free analysis of seized drugs. Bruker Applied Mass Spectrometry TN-56, 1900365 Version 2. URL: <https://bams.showpad.com/share/SznoQ4ZAsgalddeZs755G>

Nordhorn, I., Schneider, B., Groeschel, L., Kempf, J., Baessmann, C. (2024). DART-HRMS for the rapid screening of seized drugs: A study on authentic paper samples. Bruker Applied Mass Spectrometry. AMS-016 1910130. URL: <https://bams.showpad.com/share/PtTMyaxjMIMaQWFI87dp>

Please visit also Bruker's webpage for mass spectrometry-based solutions for forensic analysis at URL: <https://www.bruker.com/en/landingpages/bams/markets/forensic.html>

Contact

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Rapid Data Rationalization for Biotransformation using the Xevo MRT Mass Spectrometer with Dedicated Data-Mining Software

Ross Chawner¹, Hania Khoury-Hollins¹ Ismael Zamora² Fabien Fontaine² Martin Palmer¹ Richard Lock¹ and Jayne Kirk¹

¹Waters Corporation, Wilmslow, UK,

²Mass Analytica, Sant Cugat del Vallès, Spain

Introduction

Whilst the support of biotransformation studies using high-resolution mass spectrometry (HRMS) for structural characterization of drug metabolites is well established, key limitations exist around these approaches. Provision of fit-for-purpose HRMS data is often subject to compromise, where the interplay between mass resolving power and scan-speed brings an inherent reduction in performance, particularly when using ultra-performance liquid chromatography. In addition, providing actionable data remains challenging due to protracted data rationalization *via* manual data interrogation, often introducing bias. Here, we present a novel data-independent and data dependent workflow for metabolite characterization, utilising routine part-per billion (ppb) mass accuracy, rapid scan speeds and dedicated software to leverage these unique data attributes; in turn, reducing analytical compromise, increasing confidence and reducing time to result.

Methods

Clozapine was incubated (37 °C, t=1 h) in rat and human microsomes (20 µM with GSH (5 mM)) before termination and subsequent centrifugation. Samples were analyzed using reversed-phase UPLC separation (0.4 mL/min, C18 (2.1 x 100 mm, 1.7 µm, 40 °C)). Metabolite detection was performed in positive or negative electrospray ionization using the Xevo MRT mass spectrometer (with a mass resolving power of 100,000 FWHM, scan speeds up to 100 Hz and mass accuracy of 500 ppb). Data were acquired using the MS^E and DDA and processed using dedicated MassMetaSite software.

Preliminary Results

High-quality structural information to be gathered using MS^E and DDA with multiple phase one metabolites and glutathione adducts detected and identified with mass accuracy measurements of ≤ 500 ppb (RMS). The impact of ppb mass accuracy combined with high mass-resolution increased overall confidence in metabolite identification. When applied automatically to parent and associated fragment ions, these improvements gave quicker data rationalization and time to result in the structural elucidation of both expected and unexpected metabolites of clozapine.

Using dedicated MassMetaSite software to automatically leverage these unique data attributes, the need for extensive manual data verification is reduced markedly. Instead, this increased data confidence introduces an unsupervised aspect to this novel workflow therefore, increasing the efficiency of these biotransformation studies and their potential impact to drug discovery.

Preliminary work was also undertaken using the prototype vacuum jacketed stainless-steel LC columns coupled to Xevo MRT mass spectrometer (MS) reducing run times to 1.5 minutes, therefore increasing throughput and improving productivity without compromising data quality.

References for further reading

Waters Corporation. (2024). Xevo MRT Mass Spectrometer Brochure. May 24-12328 720008369EN Rev. A. URL: <https://www.waters.com/nextgen/us/en/library/library-details.html?documentid=720008369&t=waters-XevoMRTMassSpectrometerBrochure-720008369>

Reid, L., Daly, M. E., Gethings, L. A., Kirk, J. (2024). Metabolomics Workflow using a Xevo™ MRT Mass Spectrometer. Waters Corporation, Application Note 720008552. URL: <https://www.waters.com/nextgen/us/en/library/application-notes/2024/metabolomics-workflow-using-a-xevo-mrt-mass-spectrometer.html>

Contact

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Thermo Fisher innovation - How can you bridge the gap between discovery and the clinic?

Tony Wiklund, Technical Sales Specialist LSMS, Nordics

Thermo Fisher Scientific, Sweden

Thermo Fisher Scientific is committed to enabling our customers to make the world healthier, cleaner, and safer. The Thermo Scientific™ Stellar™ mass spectrometer (MS) exemplifies this mission by bridging the gap between groundbreaking discoveries and clinical application. Building on the unparalleled discovery capabilities of the Thermo Scientific™ Orbitrap™ Astral™ mass spectrometer, the Stellar™ MS empowers you to verify your findings with precision. It delivers innovative, targeted, and quantitative analyses that are both fast and sensitive, all while requiring minimal method development for routine operation. With the Stellar™ MS, you can seamlessly transition from discovery to clinical practice, driving forward the advancement of science and healthcare.... but can it do more?

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OAD – Oxygen attachment dissociation – A novel, unique, selective MS/MS fragmentation technology that specifically fragments at a C=C bond position

Magnus Olin, Emily Armitage,*

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Oxygen Attachment Dissociation (OAD) is a unique, selective MS/MS fragmentation technology patented by Shimadzu. It is an innovative technique that specifically breaks C=C bonds, which opens up possibilities e.g. for identifying signalling lipids in biomarker research (lipidomics, metabolomics) and charactering flavours and fragrances in the food and perfume industries.

OAD is available as an add-on to Shimadzu QTOF 9050. OAD MS/MS is a radical induced dissociation where atomic oxygen (O) and hydroxyl radicals (OH) are generated in a radical source and introduced into a collision cell instead of a collision gas effectively generating C=C specific fragmentation.

In a metabolomics study of pancreatic ductal adenocarcinoma (PDAC), potential biomarkers were identified that differentiated PDAC serum samples from healthy controls. Phospholipids represent some of the most significant differences between PDAC and healthy phenotypes. Many of the lipids contained the fatty acyl chain 18:2. OAD-MS/MS analysis revealed the same isoform with double bonds in the 6th and 9th position.

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SCIEX Advances in Mass Spectrometry for Metabolomics – 7500+, ZenoTOF and EAD fragmentation

Anders Dahl Knudsen, and Tom Ruane,

Sciex

SCIEX have long been developing LC-MS solutions for those working in the metabolomic and lipidomic research. In recent years, the use of alternative fragmentation strategies have been employed more and more in life science research. The development of EAD fragmentation with the high sensitivity ZenoTOF in particular has provided an alternative fragmentation that can assist in structural elucidation of unknown metabolites and allow for true lipid isomer quantification. High sensitivity, high quality MS² spectra (whether EAD or CID fragmentation) helps the detection of more features but also assists in translating relevant features into compound annotations – the main bottleneck for those working in untargeted metabolite ID. Good quality MS² spectra also means we can employ the benefits of accurate mass for quantification (MRM-HR) for closely related analytes in matrices with many interference – whilst maintaining sensitivity comparable to that of high end triple quadrupole based platforms. Finally, we will explore the application of SCIEX's latest triple quadrupole technology to metabolite and lipid quantification.

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Non-Targeted Analysis using comprehensive-two-dimensional gas chromatography coupled to a mass spectrometry

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Keywords: GCxGC, HRMS, POPs, NTS, Environmental

Modern society produces an increasing number of chemicals, many of which enter the environment through various pathways. Non-Target Screening (NTS) workflows using high-resolution mass spectrometry have become essential tools for identifying these contaminants in complex samples. This study demonstrates the application of comprehensive two-dimensional gas chromatography coupled with time-of-flight mass spectrometry (GCxGC-TOFMS) for enhanced separation and high-speed acquisition across the full mass range.

A systematic workflow was developed for screening both target and non-target contaminants. Identification and confirmation were achieved through native standards and targeted processing methods. Additionally, a novel Multi-Mode Source (MMS) capable of EI/CI ionization was employed, providing library-searchable spectra, accurate mass, and molecular ion data for enhanced identification confidence.

The results highlight the advantages of GCxGC in achieving superior separation and structured chromatograms, while the MMS facilitated rapid switching between ionization modes without hardware changes. This combination enabled the identification of halogenated persistent organic pollutants (POPs), pesticides, and disinfection by-products in environmental samples. The integration of ECNI spectra, EI data, and retention indices further supported compound identification.

This approach emphasizes the potential of advanced analytical techniques to address the challenges of environmental contamination, paving the way for more comprehensive monitoring and assessment of chemical pollutants.

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