AZO NETWORK

INDUSTRY FOCUS

Mass Spectrometry

An exclusive collection featuring top-tier articles, visionary experts, and essential industry insights

Sponsored by

BRUKER

November 2025 - Edition 2

TABLE OF CONTENTS

4 INSIGHTS FROM INDUSTRY

Evolution in Mass Spectrometry: Simplifying Workflows for Routine Testing

12 NEWS

Review: Key Advances Making MS Faster and Sharper

15 NEWS

Nano-Biochar Converts Toxic Silver Ions into Stable Nanoparticles within Rice Plants

19 ARTICLE

How DART-HRMS Enables Ultra-Fast Screening of Seized Drugs

30 NEWS

Eco-Friendly Nitrate to Ammonia Conversion with Trimetallic LDH Catalysts

34 NEWS

Laser-Driven Optical Mining Study Reveals How Beam Control and Mineral Makeup Unlock Asteroid Water Extraction

38 ARTICLE

How Ion Mobility-HRMS Takes PFAS Detection Beyond Regulatory Limits

51 NEWS

MassQL: A Universal Language for MS Data Analysis

54 ARTICLE

Next-Generation Mass Spectrometry Coupled with Microfluidics for Trace-Level Hazmat Analysis

Foreword

Welcome to the latest edition of our Industry Focus eBook, where we take a closer look at the fast-moving world of mass spectrometry. As one of the most powerful analytical tools in modern science, mass spectrometry continues to drive progress across a wide range of fields, from life sciences and environmental research to mining, clean tech, and materials science.

In this collection of articles, we highlight the growing impact of next-generation mass spectrometry systems, especially when combined with technologies like microfluidics. These advanced pairings are boosting trace-level detection of hazardous materials and enabling faster, more accurate analyses in critical areas such as homeland security, public health, and forensic science.

Ongoing advancements in miniaturization, automation, and resolution are reshaping how researchers approach chemical and biological analysis. From exploring optical methods for ion beam profiling to applying high-resolution mass spectrometry in mining operations, or detecting emerging environmental contaminants with increased sensitivity, each innovation demonstrates the expanding versatility of the technique.

You'll also find insight into how mass spectrometry supports sustainable technologies, identifying pollutants in water and air, and aiding developments in green chemistry. In materials science, it's playing a vital role in uncovering atomic-level details that inform the design of novel alloys and advanced composites.

Looking ahead, this eBook explores how artificial intelligence and machine learning are starting to influence the interpretation of mass spectrometry data, speeding up discovery and opening up new possibilities for research and application.

As you explore these pages, we invite you to consider how mass spectrometry is shaping today's interdisciplinary research landscape. Whether you're an experienced analyst or just beginning to explore the field, we hope this curated collection provides valuable insights into where the science is going, and the innovations helping to drive it forward

Evolution in Mass Spectrometry: Simplifying Workflows for Routine Testing

In this interview, AZoM speaks to Jeff Zonderman from Bruker Applied Mass Spectrometry about the future of mass spectrometry, and the tools and technologies that will transform research.

Could you provide some insights into your background and how you became involved in developing mass spectrometry solutions?

I am Jeff Zonderman, Senior Vice President of the Applied Mass Spectrometry Division of Bruker I have been involved in mass spectrometry and chromatography for over 30 years.

Initially, I worked as a DNA synthesis chemist. I began using mass spectrometry, specifically MALDI mass spectrometry, to analyze oligonucleotides for quality control instead of chromatography, which I found much easier. As a synthetic chemist, I quickly developed a strong interest in mass spectrometry and the valuable information it provided.

My career path eventually led me into mass spectrometry sales, where I worked across various areas and technologies.

I then became CEO of IonSense, which pioneered ambient ionization. Three years ago, Bruker acquired IonSense and its technology; Direct Analysis in Real-Time (DART) mass spectrometry.

As Senior Vice President of Bruker Applied MS, what are the key objectives driving the development of products like the EVOQ DART-TQ⁺? How does this instrument address the challenges faced in routine testing?

We established our new division, Bruker Applied Mass Spectrometry, to address the specific needs of the applied markets for mass spectrometers. Bruker has already followed a similar path with the MALDI Biotyper , transforming a mass spectrometer by simplifying the workflow, removing chromatography, and creating the most widely used clinical mass spectrometer on the market.

We are taking a similar approach for our new Bruker Applied MS division, focusing on technologies like triple quadrupole and QTOF and simplifying workflows. One of our main objectives is to develop products that streamline workflows.

We aim to develop chromatography-free workflows that are simpler, more robust and sustainable by reducing large amounts of organic waste.

This simplification also benefits users in applied markets who may not be experts in mass spectrometry, enabling broader access to the technology.

The EVOQ DART-TQ$^+$ is the first triple quadrupole MS system designed for DART ion source plug-and-play operation. What benefits does this offer for routine laboratory environments, and how does this compare to traditional workflows?

With DART integrated into a quantitative workflow and chromatography removed, we address several key laboratory areas. First, eliminating chromatography removes much of the complexity associated with maintaining LC instrument uptime and user training, greatly simplifying the workflow.

Removing the chromatography step with DART technology significantly reduces the cost of ownership, including the costs associated with consumables and operational waste.

Reducing organic solvent use is also a significant benefit, supporting Bruker's commitment to sustainability, as many companies prioritize minimizing environmental impact today.

The EVOQ DART-TQ$^+$ is highlighted for its chromatography-free workflows. Could you explain how the instrument achieves these workflows and the key technological advancements enable it?

The primary technological advancement in the EVOQ DART-TQ$^+$, DART is an ambient ionization technique that ionizes samples with a gas flow instead of a liquid flow.

This approach makes the workflow far more robust and significantly faster. We eliminate the separation time by removing chromatography, allowing for high-throughput quantitative analysis. Without chromatography, analysis time for quantifying target analytes goes from minutes to seconds.

Image Credit: PeopleImages.com - Yuri A/Shutterstock.com

The EVOQ DART-TQ$^+$ allows for quick switching to LCMS. Why is this ability important, and how does it compare to conventional methods?

While we emphasize a chromatography-free approach, the specific application must be considered. Some workflows will still require chromatography.

The EVOQ DART-TQ$^+$ is an excellent triple quadrupole mass spectrometer with and without DART, offering high sensitivity, selectivity, and robustness in electrospray mode. It is unlikely that every method will become chromatography-free overnight; this is an ongoing process.

DART is very effective for targeted, high-throughput assays, but some applications still need chromatography. The EVOQ DART-TQ$^+$ system allows easy switching between DART and LCMS modes, with ion source changes taking only a minute or so. Thus, the system provides the flexibility to leverage both techniques as needed.

In addition to lowering the cost per sample, does the chromatography-free workflow provide other financial benefits?

Yes. Eliminating LC system maintenance and downtime as well as another major financial benefit is eliminating high disposal costs for organic waste. This aligns with a significant demand from our customers, who increasingly seek evidence that we prioritize sustainability as a company.

Bruker is strongly committed to ESG and sustainability initiatives, and this reduction in waste from routine workflows is a clear example.

Chromatography-based mass spectrometry processes typically generate large amounts of organic waste, but by removing chromatography, we can minimize that waste, demonstrating our dedication to enhancing the sustainability of our products.

Can we expect to see other chromatography-free frameworks at Bruker in other application areas?

The triple quadrupole system was our first fully integrated product to showcase DART technology after Bruker acquired IonSense. However, we utilize DART across various mass spectrometers.

For instance, we integrate DART with our QTOF systems and timsTOF technology, which is especially exciting. In some applications, separation—such as the separation of isomers—may still be necessary. By pairing DART with timsTOF ion mobility, we are developing new, highly effective workflows. Ion mobility can often serve as a substitute for chromatography in achieving separation.

This approach also allows us to move beyond quantitative methods and routine analysis in triple quads to platforms with ion mobility. The timsTOF system is a prime example of this advancement.

Image Credit: Bruker Applied Mass Spectrometry

You have emphasized the importance of making routine testing easier and more cost-effective. Besides the instrumentation advances you have discussed, what other areas of development are Bruker Applied MS working on to support customers?

We are focusing on all areas of the workflow. We have developed software for targeted and untargeted database searching and implementation for quantitative mass spectrometry.

This backend software includes databases and processing tools. We also invest in the front end by developing kits and forming partnerships with companies such as Pinpoint Testing, a forensics toxicology firm, to provide complete workflow solutions. We are also enhancing automation systems to streamline sample extraction and spotting onto our sample screens, allowing for efficient sample handling in the mass spectrometer.

In summary, we are making strategic investments across the entire workflow, including kit

development, partnerships, front-end automation, and integration of DART and other techniques with our mass spectrometers. Ultimately, the goal is to deliver quick, cost-effective, and reliable reporting.

What exciting plans does Bruker Applied MS have in the pipeline?

Several exciting developments are underway, particularly around integrating DART technology and other advanced techniques with our mass spectrometers to create complete workflows.

I am especially enthusiastic about the potential of combining DART ion mobility with our timsTOF for a range of applications and the DART triple quad system for high-throughput quantitative analysis. Bruker is investing heavily in the applied markets, so you can expect many future innovations.

About the Speaker

Jeffrey Zonderman serves as the Senior Vice President of Bruker Applied Mass Spectrometry, a new division of the company focused on providing mass spectrometry-based solutions for the applied market segments such as forensics, food, environmental, industrial/polymer, and clinical research. Jeffrey graduated from Northeastern University with a bachelor's in biology and has been involved in mass spectrometry and chromatography for over 30 years. Before joining Bruker, Jeffrey worked in applications, sales/marketing and general management roles. His previous position was CEO of IonSense Inc, a company focusing on ambient ionization technology and commercialized DART (Direct Analysis in Real Time) technology. As Senior VP of Bruker Applied MS, Jeffrey looks to expand the applications of DART technology, amongst others, for chromatography-free mass spectrometry-based workflows.

This information has been sourced, reviewed and adapted from materials provided by Bruker.

For more information on this source, please visit Bruker.

Review: Key Advances Making MS Faster and Sharper

Breakthroughs in laser control, ion optics, and multimodal imaging are turning mass spectrometry imaging into one of science's most precise molecular mapping tools.

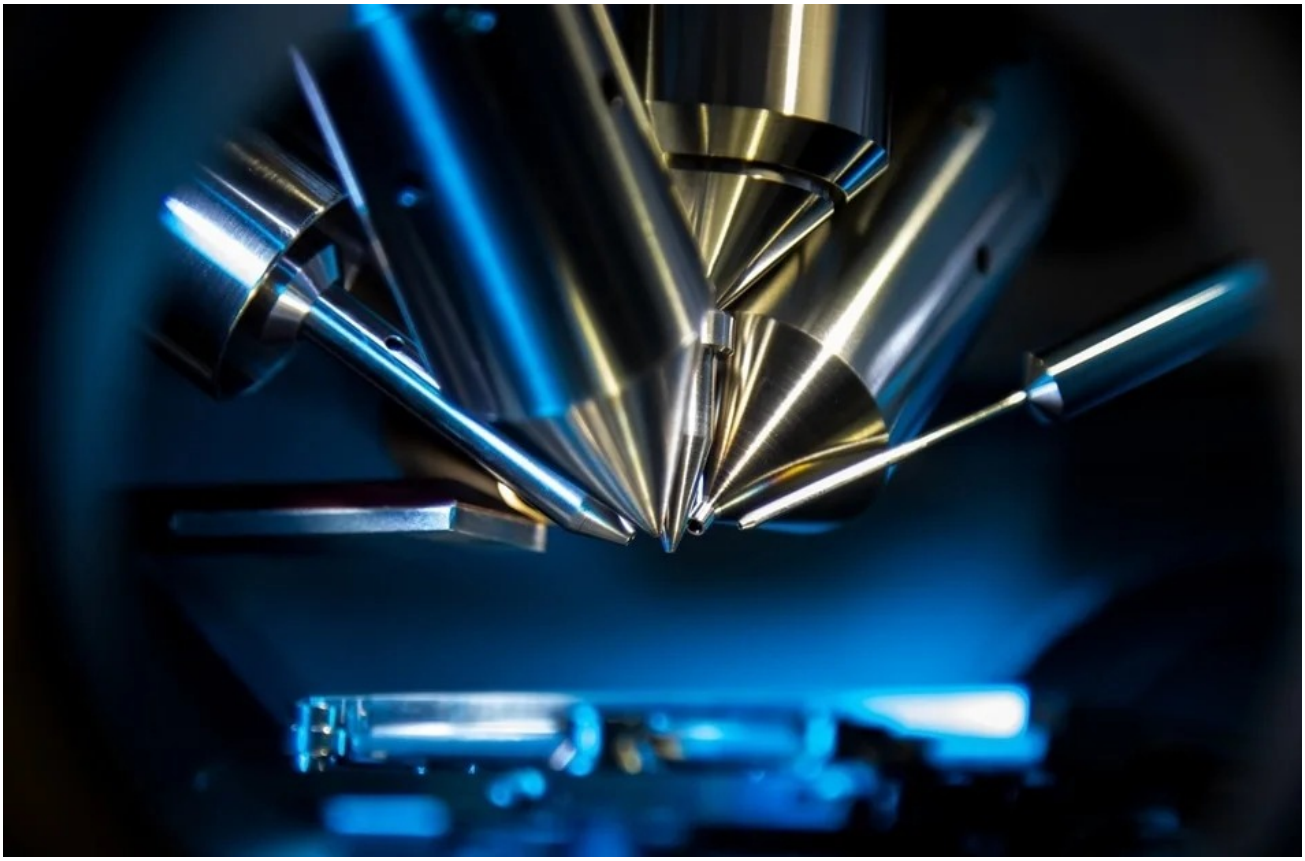


Image Credit: Intothelight Photography/Shutterstock.com

A new review in *Analytical Chemistry* from researchers at Maastricht University and collaborators outlines how a combination of optical, ionization, and instrumental innovations is driving the next generation of Mass Spectrometry Imaging (MSI).

The Study

Their paper explores progress across laser- and ion-based methods, such as MALDI, SIMS, LA-ICP, and LAESI, and highlights how improvements in beam control, detector speed, and ion optics are refining MSI's spatial precision, sensitivity, and throughput.

MSI works by directing a focused laser or ion beam onto a sample surface to desorb and ionize molecules, capturing the resulting ions in a mass spectrometer to produce molecular maps.

Each pixel represents a complete mass spectrum, enabling scientists to visualize chemical distributions without labeling.

Methods like Matrix-Assisted Laser Desorption/Ionization (MALDI) rely on a co-crystallized matrix that absorbs laser energy and aids ionization, while Secondary Ion Mass Spectrometry (SIMS) uses a primary ion beam for high-resolution elemental mapping.

The review also explored variants such as Laser Ablation Inductively Coupled Plasma (LA-ICP), Laser Ablation Electrospray Ionization (LAESI), and Desorption Electrospray Ionization (DESI), which extend MSI into elemental, ambient, and matrix-free domains.

Advances So Far

Spatial resolution in MSI continues to improve through advances in laser focusing and beam geometry. The review details the distinction between microprobe and microscope acquisition modes, where there is a trade-off between throughput and spatial precision.

Recent studies refining optics, including reflection and transmission geometries, aspherical lenses, beam homogenizers, and diffraction gratings, have facilitated spot sizes down to the micrometer scale. These developments are critical for mapping cellular heterogeneity and drug distribution in tissues.

Another recent breakthrough, MALDI-2 post-ionization, boosts ion yields by two to three orders of magnitude, pushing imaging below the one-micrometer threshold. Combined with ultrafast femtosecond and picosecond laser systems, these methods allow gentler ablation and reduced thermal damage, which is particularly valuable for analyzing sensitive biological structures.

Improvements in detector design and ion mobility spectrometry are also enhancing molecular specificity and reducing spectral overlap, while cryogenic SIMS (cryo-SIMS) and 3D MSI approaches preserve fragile species and reveal spatial organization in three dimensions.

Going Forward

The review emphasized that MSI's progress now extends beyond optics. New hardware designs and data acquisition strategies have drastically increased imaging speed, while multimodal methods that combine MSI with optical and electron microscopy are facilitating richer, more

spatially aligned datasets.

Together, these advances are transforming MSI from a specialized analytical tool into a platform capable of comprehensive molecular imaging at cellular and subcellular levels.

By integrating complementary techniques, such as imaging mass cytometry (IMC) and multiplexed ion beam imaging (MIBI), and using faster detectors, improved throughput, and 3D reconstruction workflows, MSI is rapidly maturing into a high-resolution, high-sensitivity system for biomedical and materials research.

The authors concluded that continued collaboration among chemists, physicists, and biologists will be key to pushing the limits of this powerful technology even further.

Journal Reference

Körber, A., *et al.* (2025). Mass Spectrometry Imaging. *Analytical Chemistry* 15517, 97. DOI: 10.1021/acs.analchem.4c05249, https://pubs.acs.org/doi/full/10.1021/acs.analchem.4c05249

Nano-Biochar Converts Toxic Silver Ions into Stable Nanoparticles within Rice Plants

By triggering silver nanoparticle formation inside rice plants, scientists have revealed how nano-biochar actively shapes metal movement in soil, and what that means for food and environmental safety.

Image Credit: waragon injan/Shutterstock.com

Researchers at Hebei University of Technology have discovered an unexpected new function for nano-biochar, demonstrating its ability to promote the natural creation and buildup of silver nanoparticles within rice roots.

The research, published in *Biochar*, illustrates how this minuscule carbon substance engages with plant roots to convert silver ions into metallic nanoparticles, which may influence plant health and the transport of metals in the environment.

Silver is used extensively in electronics, medicine, and antimicrobial products, resulting in the discharge of silver ions into soils and water bodies. These ions exhibit high reactivity and may present dangers to living organisms. In contrast, silver nanoparticles are more stable and

exhibit lower toxicity. However, the natural formation of these particles in soils has not been well understood.

Led by Shiguo Gu and Fei Lian from Hebei University of Technology, the research team found that nano-biochar functions as an electron shuttle within the rhizosphere, the confined area of soil that encircles plant roots.

When introduced into soil around the rice plants, the nano-biochar particles facilitated the transfer of electrons to the oxygen released from the roots. This mechanism produced superoxide radicals, which subsequently reduced silver ions, resulting in the formation of silver nanoparticles. The presence of the superoxide radicals was confirmed through specialized probe and quenching experiments.

The team used high-resolution microscopy and single-particle ICP-MS to verify that the nanoparticles developed around the roots and accumulated within the rice leaves and cells.

Interestingly, a moderate quantity of nano-biochar facilitated the formation of silver nanoparticles, whereas excessive quantities diminished oxygen secretion from roots and inhibited the process. The team linked this inhibitory effect to excess nano-biochar covering root surfaces and interfering with oxygen release through the aerenchyma tissues.

The researchers also discovered that nano-biochar decreased rice's overall uptake of toxic silver ions while enabling the accumulation of less toxic nanoparticles in both roots and shoots. This finding indicates that nano-biochar can safeguard plants from toxic metals and affect the movement of metals within the soil-plant system.

> *“Our findings highlight that nano-biochar is not just a passive soil amendment but an active participant in chemical transformations in the rhizosphere. It plays a catalytic role in regulating redox-active metals and could influence how these elements cycle through ecosystems.*
>
> *Fei Lian, Hebei University of Technology*

The research introduces new inquiries regarding the possibility of naturally occurring nanoparticles infiltrating the food chain. At the same time, it presents opportunities to use the reactivity of biochar to enhance soil health and promote sustainable agricultural methods.

The authors propose that comprehending and regulating nano-biochar's dual impacts, its capacity to detoxify metals while facilitating nanoparticle formation, will be essential to guaranteeing environmental safety and food security.

Journal Reference:

Gu, S., *et al.* (2025) Insight into the crucial role of nano-biochar in the natural formation and bioaccumulation of silver nanoparticles in the rhizosphere by single-particle ICP-MS. *Biochar*. doi.org/10.1007/s42773-025-00492-w

---

Source:

- Hebei University of Technology

EVOQ® DART-TQ+

Unlock the Future of Mass Spectrometry with EVOQ® DART-TQ+

Introducing the EVOQ® DART-TQ+, the groundbreaking triple quadrupole mass spectrometer designed to transform your laboratory's efficiency and productivity. With the first and only fully integrated Direct Analysis in Real Time (DART) ion source, this breakthrough system is built for reliable, routine analysis, delivering exceptional triple quadrupole analytical performance day in and day out.

Speed and Precision

At the heart of the EVOQ® DART-TQ+ is its advanced electronics, engineered to generate high-quality data for rapid, high-throughput analysis. With extremely rapid MRM transitions and the ability to monitor more compounds in less time, this system guarantees extraordinary ion transmission from the smallest ion to the maximum mass range. Whether you're running efficient chromatography-free workflows or conventional LC-MS workflows, the EVOQ® DART-TQ+ provides fast acquisition, sustained sensitivity, and robustness.

Efficiency and Cost-Effectiveness

Designed for straightforward routine assay workflows, the EVOQ® DART-TQ+ enables rapid screening and confirmation of samples with cost-effective chromatography-free workflows. Increase sample throughput, lower operational costs, and enjoy fast result generation with high uptime. The system's turnkey software streamlines sample acquisition to report, enhancing lab efficiency and productivity.

Environmental Responsibility

Bruker, the innovative company behind EVOQ® DART-TQ+, is committed to sustainability. The system's green-enabled features reduce energy and solvent consumption, minimizing waste and supporting a more sustainable future. With sensitivity to spare, reliability, accuracy, and precision, the EVOQ® DART-TQ+ ensures compliance with regulatory standards, protecting human health and ecosystems.

Experience the EVOQ® DART-TQ+

Join the future of mass spectrometry with the EVOQ® DART-TQ+. See it in action and discover how this innovative system can revolutionize your laboratory's operations.

For more information, please visit: bruker.com/evoq-dart-tq

How DART-HRMS Enables Ultra-Fast Screening of Seized Drugs

Increased backlogs of seized drug samples, rapid turnaround times, and the emergence of many novel psychoactive substances (NPS) are major challenges for the forensic community worldwide.

This article demonstrates a comprehensive workflow provided by the Seized Drug Suite, which incorporates the powerful combination of Direct Analysis in Real Time and High Resolution Mass Spectrometry (DART-HRMS).

This unparalleled pairing combines ultra-fast acquisition speed with high information depth for targeted and non-target analyses.

Introduction

An ever-increasing number of seized drug samples, as well as a constant influx of novel psychoactive substances, pose challenges to forensic labs around the world.

The NFLIS-Drug 2019 Survey of Crime Laboratory Drug Chemistry Sections Report revealed that laboratories have an average turnaround time of 60 days and a backlog of 1,800 drug cases.[1] This demonstrates that established conventional techniques are being pushed to their limits by the current demand for sample throughput.

A potential alternative is to use Direct Analysis in Real Time in combination with High Resolution Mass Spectrometry (DART-HRMS) for screening analysis. Early adopters have already praised DART-MS for its ability to produce reliable analytical results much faster and more easily than traditional techniques.[2]

What has been lacking so far is the seamless integration of DART into routine testing workflows.

This article demonstrates the use of DART-HRMS to investigate paper samples seized during routine controls in prisons and forensic psychiatry institutions. A common method of smuggling drugs into prison involves soaking letter-writing paper in a drug mixture, allowing it to dry, and then writing on it.

The prisoner receives the letter and reads it, then smokes portions of it to consume the drug.

To counteract this approach, authorities have developed methods for screening letters sent into prison.

Fast Seized Drug Screening with the Seized Drug Suite

Analysis of Authentic Paper Samples

The Seized Drug Suite was used to screen paper samples seized during routine controls in prisons and forensic psychiatric institutions. The Seized Drug Suite is a hardware and software package that includes optimized methods for acquisition, processing, and reporting designed specifically for the analysis of seized drug samples.

The samples were extracted with MeOH and 3 µL of the extract was placed on a DART QuickStrip® card. All analyses were performed using a DART JumpShot® source and a compact QTOF mass spectrometer (both from Bruker).

Helium was used as an ionization gas at 275 degrees Celsius. Data was collected in positive ionization mode with AutoMS/MS at 24 eV and 36 eV collision energies.

TargetScreener HR was used for subsequent LC-MS confirmation analysis after an Elute UHPLC was connected to the compact QTOF instrument. The simple exchange from the DART source to the Vacuum Insulated Probe-Heated ElectroSpray Ionization (VIP-HESI) source takes only a few minutes and does not break the vacuum.

Data Acquisition

The Bruker compact QTOF instrument's fast data acquisition speed enables it to receive full scan MS information as well as MS/MS fragmentation spectra within the DART analysis's very short run time, which is typically 3 s to 60 s.

During the acquisition, the compact QTOF mass spectrometer switches between MS and data-dependent AutoMS/MS at high collision energy. AutoMS/MS parameters were carefully tuned to obtain high-quality fragment data on the most selected precursors.

The "active exclusion" parameter ensures fragmentation of low-abundant precursor ions in the presence of hi-abundant precursors enabling maximum coverage of precursor ions selected for MS/MS.

Spectral Library Search

Spectral library searches help identify compounds. An open library concept allows libraries to

be chosen freely and integrated into the workflow. The Seized Drug Suite includes a spectral library containing MS/MS spectra for over 280 compounds obtained using DART-QTOF-MS.

Because there is no significant difference in fragmentation patterns between DART and ESI, there is no reason to use only DART-specific libraries. In addition, custom spectral libraries can be built and modified.

The NIST DART-MS Forensic Database (2021), the "Maurer, Meyer, Helfer, Weber: LC-HR-MS/MS Library of Drugs, Poisons, and Their Metabolites" and the NIST/EPA/NIH Mass Spectral Library 2023 are among the libraries available.

Sample Report

The sample report is generated automatically and contains all relevant information, such as a data table with sample and method information, an overview of the library search results, and spectral details for each compound found.

Image Credit: Bruker Applied Mass Spectrometry

Overview Of the Sample Preparation Process, Hardware and Software Used

Figure 1. *Overview of the sample preparation process, hardware and software applied. Image Credit: Bruker Applied Mass Spectrometry*

Workflow for Screening of Seized Drug Samples with DART-HRMS/MS

Full scan MS and data-dependent MS/MS information are acquired in parallel. A sample analysis time of 12 seconds results in up to 120 MS/MS spectra.

TargetScreener is used for confirmation of the results (see Figure 2). It provides a comprehensive screening solution, including a high-quality, regularly updated forensic database of over 1,000 compounds with forensic relevance.

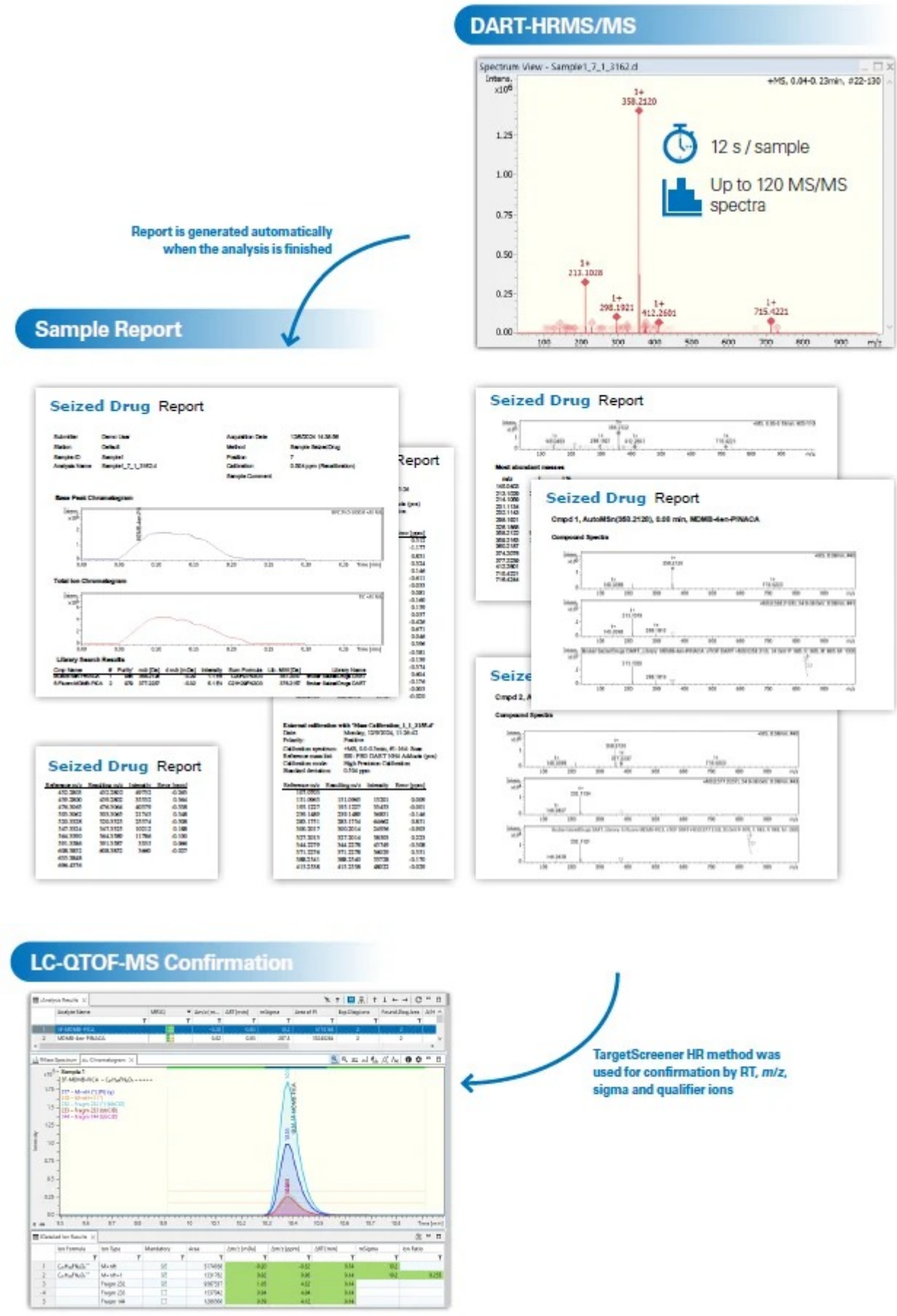


Figure 2. *Workflow for screening of seized drug samples using DART-HRMS. Image Credit: Bruker*

Results

Authentic paper samples were analyzed using the Seized Drug Suite workflow. Figure 2 shows the results for one selected paper sample. Data acquisition was completed in 12 seconds, yielding approximately 120 individual MS/MS spectra.

Two synthetic cannabinoids, MDMB-4-en-PINACA and 5-Fluoro-MDMB-PICA, were successfully identified using library match scores greater than 900. Both were later confirmed through LC-QTOF-MS analysis. Synthetic cannabinoids were identified as the dominant drug effect group across all analyzed paper samples.

This group includes substances that function similarly to THC (d9-tetrahydrocannabinol) in that they interact with cannabinoid receptors. In recent years, synthetic cannabinoids have taken the lead among NPS. From December 2021 to May 2023, 40% of newly reported NPS were synthetic cannabinoids.[3]

As of 2022, MDMB-4-en-PINACA was the most frequently reported synthetic cannabinoid in the United States, with 5-Fluoro-MDMB-PICA ranking third.[4]

Identification of Unknowns

With the constant emergence of these NPS, it is common for seized drug samples to produce signals that do not match any existing library entries but may still be forensically relevant. Another significant advantage of high-resolution mass spectrometers is their ability to identify unknown compounds.

QTOF mass spectrometers measure the mass of an ion with greater accuracy than low-resolution instruments such as quadrupoles, allowing for the determination of the elemental composition of unknown compounds.

Matching the experimental isotope pattern of the discovered elemental composition to the theoretical one provides a second criterion for validating the formula prediction.

MS/MS fragmentation spectra provide structural information that can be compared to *in-silico* fragmentation patterns of compound structures found in databases. As a result, compound identification can be narrowed down step by step using these three criteria.

MetaboScape®, Bruker's software, guides the user through a seamless three-step workflow from initial spectral features to final annotations in an automated and efficient manner. Below is a detailed walkthrough of this process, with the annotation of the synthetic cannabinoid ADB-BUTINACA as an example.

First, MetaboScape's SmartFormula tool lists the best-matching elemental compositions based on the calculated accurate mass and isotope patterns. Here, the user can specify which elements should be considered.

In the following step, the CompoundCrawler tool searches publicly available databases like PubChem and a local, customizable database called AnalyteDB for structure candidates that correspond to the elemental compositions.

To address the issue of structures having to be listed in public databases for CompoundCrawler to detect them, AnalyteDB allows users to incorporate their own structures directly at the local level. Such new structures could be derived from deep learning or AI-based predictions.

As a final step, the discovered structure candidates are suspected of in-silico fragmentation by MetFrag[5] and compared to the experimental MS/MS spectrum. The workflow described here represents a standard-free annotation approach by utilizing in-silico fragmentation.

This is especially useful for NPS, where reference standards are not always readily available. After successfully identifying a new compound, it can be saved in the spectral library for future comparisons and searches.

Using the principle of 'all data is collected all the time', retrospective evaluation of previously analyzed samples is possible without repeating any experimental work.

Three-Step Workflow for the Unknown Annotation in Metaboscape.

The identification of ADB-BUTINACA without the need for a standard is presented below.

SmartFormula

SmartFormula calculates possible elemental compositions based on isotope pattern fit and m/z measurements.

CompoundCrawler

CompoundCrawler looks for structure candidates among the proposed elemental compositions.

MetFrag

MetFrag fragments structure candidates *in-silico* and compares the results to the experimental MS/MS spectrum.

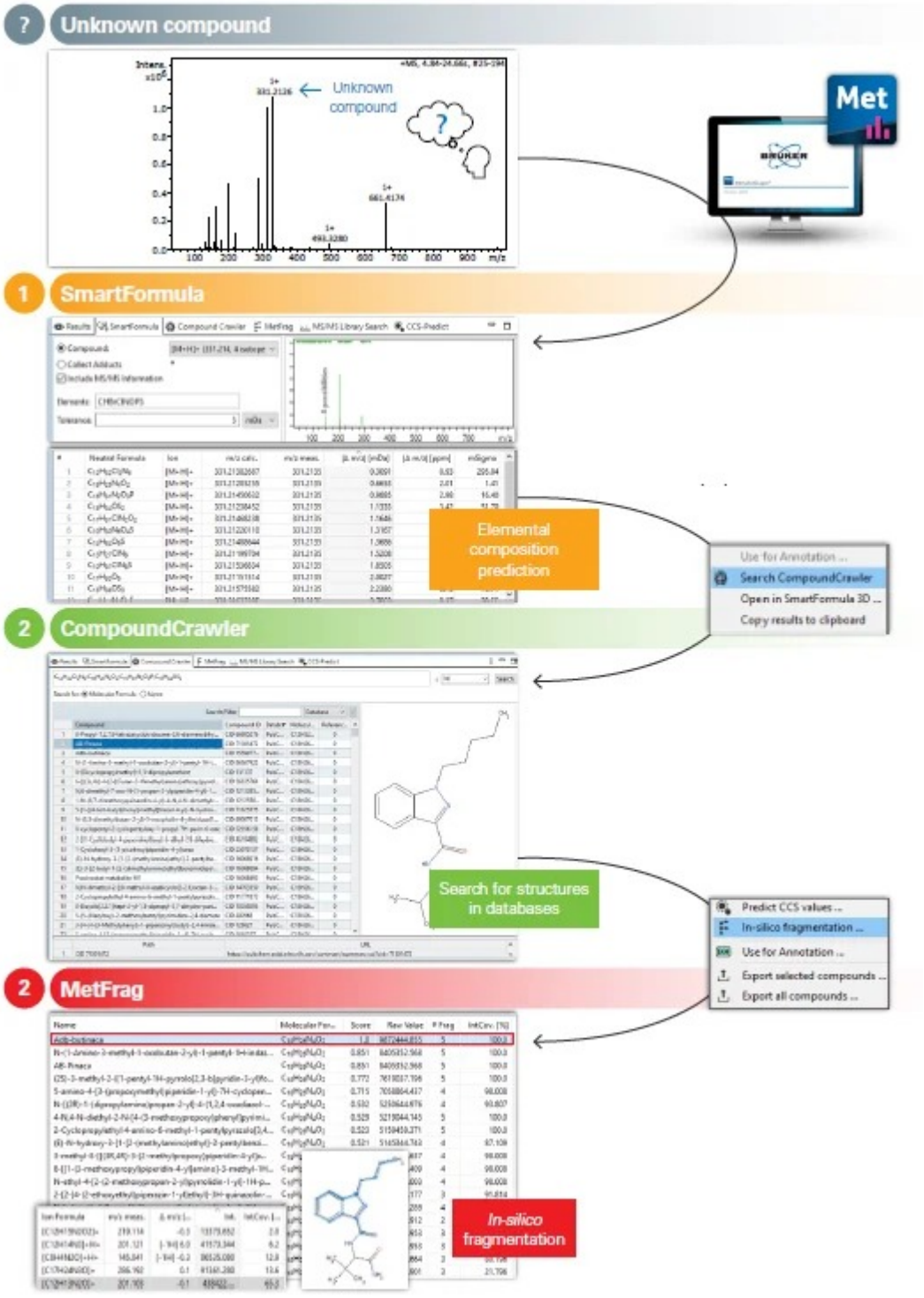


Image Credit: Bruker Applied Mass Spectrometry

Differentiation of Isomeric Synthetic Cannabinoids

Differentiating between isomeric drugs is critical for accurate identification. While chromatography-free methods do not rely on retention time separation, DART-QTOF-MS can effectively distinguish isomeric drugs in various situations by analyzing their fragmentation profiles.

ADB-BUTINACA and AB-PINACA are isomeric synthetic cannabinoids with the same chemical formula $C_{18}H_{26}N_4O_2$.

The only structural difference between these compounds is the position of one methyl group. This minor structural difference, however, is sufficient to distinguish them using DART-HRMS/MS based on fragmentation patterns.

The methyl-group in ADB-BUTINACA is located at the part of the molecule that causes the neutral loss, whereas in AB-PINACA, it is located at the detectable fragment ion.

A characteristic fragment ion at m/z 201 and 215 is thus observed, which serves to differentiate the two isomers. The identification of ADB-BUTINACA in the seized paper sample shown in Figure 3 is unambiguous because the fragment ion at m/z 201 was detected.

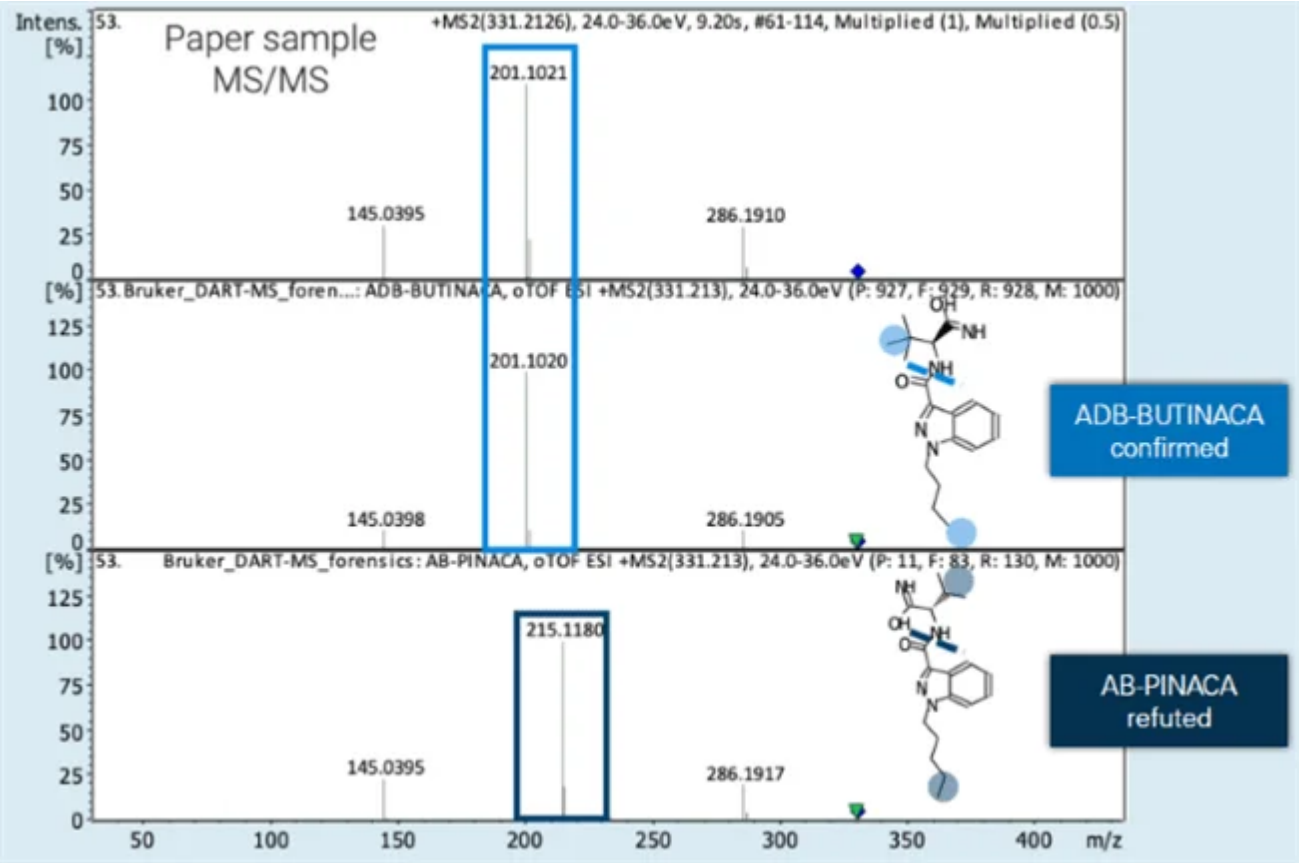


Figure 3. *Differentiation of the isomeric synthetic cannabinoids ADB-BUTINACA and AB-PINACA based on their fragmentation pattern. Reference standard-based identification of ADB-BUTINACA in an authentic paper sample. Image Credit: Bruker Applied Mass Spectrometry*

Conclusion

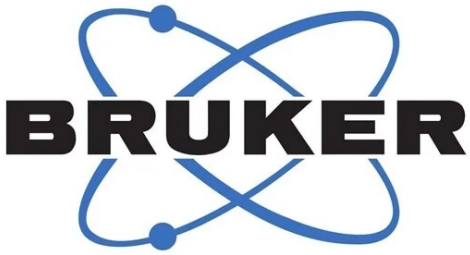
DART-HRMS was suitable for a highly accelerated screening of seized drug samples. It offers a viable alternative to traditional techniques that eliminates the need for time-consuming chromatography.

Going chromatography-free with DART saves analysis time per sample to less than a minute and significantly reduces solvent consumption. Bruker's QTOF mass spectrometer combines high detection selectivity with excellent sensitivity.

It can be used for more than just targeted analyses, such as detecting unexpected compounds or identifying unknown compounds. Because it is always in full scan mode, it makes retrospective analysis of any type of investigated sample easier, which is especially useful in the context of NPS.

References

1. U.S. Drug Enforcement Administration, Diversion Control Division. (2019). NFLIS-Drug 2019 Survey of Crime Laboratory Drug Chemistry Sections Report. Springfield, VA: U.S. Drug Enforcement Administration
2. Sisco, E. and Forbes, T.P. (2021). Forensic applications of DART-MS: A review of recent literature. *Forensic Chemistry*, 22, p.100294. https://doi.org/10.1016/j.forc.2020.100294.
3. United Nations Office on Drugs and Crime, *Current NPS Threats*, Volume VI, August 2023. Available at: https://www.unodc.org/res/scientists/ewa/Current_NPS_Threats_VI.pdf.
4. EMERGING THREAT REPORT Annual 2022 Drug Enforcement Administration Special Testing and Research Laboratory. Available at: https://cesar.umd.edu/sites/cesar.umd.edu/files/pubs/DEA-Emerging-Threat-Report-2022-Annual.pdf (Accessed 13 May 2025).
5. Wolf, S., *et al*. (2010). In silico fragmentation for computer assisted identification of metabolite mass spectra. *BMC Bioinformatics*, 11(1). https://doi.org/10.1186/1471-2105-11-148.



This information has been sourced, reviewed and adapted from materials provided by Bruker Applied Mass Spectrometry, developed in collaboration with the University of Freiburg.

For more information on this source, please visit Bruker Applied Mass Spectrometry.

Eco-Friendly Nitrate to Ammonia Conversion with Trimetallic LDH Catalysts

Researchers have introduced a novel approach for the electroreduction of nitrate (NO_3^-) to ammonia (NH_3) using layered double hydroxide (LDH) nanosheets. Their study, published in the journal *Advanced Functional Materials*, highlights how modulating surface-active hydrogen species (H*) enhances the efficiency of this process, which is crucial for sustainable nitrogen management and addressing environmental pollution.

Image Credit: Niwat panket/Shutterstock.com

The findings offer a cleaner and efficient alternative to the traditional synthesis process, paving the way for environmentally friendly nitrogen fixation in agriculture and industry.

Challenges in Conventional Ammonia Production

NH3 is essential for agriculture, electronics, and pharmaceuticals. Traditionally, it has been produced through the Haber-Bosch (HB) process, which, although effective, is energy-

intensive and produces significant carbon dioxide (CO_2) emissions. This process emits about 1.8 tons of CO_2 for every ton of NH_3. This environmental challenge has intensified the need for cleaner, more sustainable alternatives. The conventional process consumes nearly 1-2% of the world's total energy supply, highlighting the urgency for innovative solutions.

In this context, one promising method is the electrochemical reduction of NO_3^- to NH_3, powered by renewable electricity. This process reduces the carbon footprint associated with conventional synthesis and mitigates nitrate pollution in water bodies. The nitrate reduction reaction (NitRR) converts harmful NO_3^- into valuable NH_3 while contributing to the restoration of the nitrogen cycle. However, its efficiency heavily relies on the design of high-performance electrocatalysts, which determines reaction rates.

Development of Trimetallic LDH Catalysts for Electroreduction

Researchers synthesized and analyzed trimetallic NiCuFe (nickel (Ni), copper (Cu), and iron (Fe)) LDH nanosheets to enhance the electroreduction of NO_3^- to NH_3. These nanosheets were fabricated using an electrodeposition technique, where nickel foam served as the substrate and a Ni, Cu, and Fe nitrate electrolyte was employed in a 1:1:1 molar ratio. The resulting 9.9 nm-thick nanosheets featured a large surface area of 127.4 m^2/g and a three-dimensional structure that increased active site exposure and improved efficiency.

Characterization using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and energy dispersive spectroscopy (EDS) confirmed their uniform composition and morphology. Electrochemical tests conducted in a customized H-type electrochemical cell measured current density, Faradaic efficiency (FE), and NH_3 yield rate under varying potentials and NO_3^- concentrations.

The NiCuFe-LDHs demonstrated superior catalytic activity and selectivity compared to bimetallic catalysts (CuFe-LDHs and NiFe-LDHs) due to the synergistic effects of Ni, Cu, and Fe. Notably, Ni played a critical role in promoting the adsorption of hydrogen species (H*), which is essential for facilitating NitRR.

Performance Metrics of NiCuFe-LDHs

The NiCuFe-LDHs nanosheets achieved an NH_3 yield rate of 1.64 mmol h^{-1} cm^{-2} and a high FE of 94.8% at a potential of -0.4 V versus the reversible hydrogen electrode (RHE). This performance surpassed that of bimetallic catalysts, with the NH_3 FE being 1.3 times higher than CuFe-LDHs and 2.7 times higher than NiFe-LDHs. These results highlight the strong

interaction among Ni, Cu, and Fe in facilitating the NitRR while minimizing byproducts.

Operando electrochemical impedance spectroscopy (EIS) and differential electrochemical mass spectrometry (DEMS) demonstrated that Ni and Cu sites served as key active centers for the adsorption and activation of nitrate intermediates, accelerating reaction kinetics. The incorporation of Ni effectively suppressed competing hydrogen evolution reactions (HER), further improving selectivity toward NH_3 production.

Durability tests over 15 consecutive cycles confirmed the long-term stability of the NiCuFe-LDHs, maintaining an NH_3 yield above 90%. Additionally, the study highlighted that the catalyst retained structural integrity and performance even after extensive cycling. Researchers proposed integrating these nanosheets into a Zn-NO_3^- battery system, which could simultaneously treat nitrate pollutants, generate NH_3, and provide energy output.

Applications for Sustainable Nitrogen Management

This research has significant implications for sustainable nitrogen management. The ability to efficiently convert NO_3^- into NH_3 using renewable energy supports global goals to reduce carbon emissions and promote environmentally friendly agricultural practices.

The developed NiCuFe-LDHs can be implemented in future electrocatalyst designs to reduce nitrogenous compounds in wastewater treatment. Integrating this technology into energy storage systems, such as Zn-NO_3—batteries, presents an innovative dual-function approach that enables pollutant remediation and power generation.

This research addresses environmental pollution and sustainable fertilizer production by transforming harmful nitrates into valuable NH_3. It also demonstrates how renewable-powered systems can make chemical manufacturing cleaner and more efficient.

Conclusion and Future Directions

This study demonstrates the potential of trimetallic NiCuFe-LDHs nanosheets as efficient electrocatalysts for reducing NO_3—to NH_3. The nanosheets achieved high NH_3 yield and FE, marking a significant step forward in sustainable NH3 production.

Future work should focus on optimizing the composition and structure of LDHs to enhance catalytic activity and selectivity. Additionally, scaling up the synthesis process and testing the catalysts under real-world conditions will be essential for industrial applications.

Overall, this research provides a strong foundation for developing next-generation clean technology solutions that simultaneously integrate renewable energy with efficient nitrogen conversion, paving the way for a more sustainable chemical industry.

Journal Reference

Liu, B., & *et al*. (2025). Modulating Surface-Active Hydrogen for Facilitating Nitrate-to-Ammonia Electroreduction on Layered Double Hydroxides Nanosheets. Advanced Functional Materials, e19238. DOI: 10.1002/adfm.202519238. https://advanced.onlinelibrary.wiley.com/doi/10.1002/adfm.202519238

Laser-Driven Optical Mining Study Reveals How Beam Control and Mineral Makeup Unlock Asteroid Water Extraction

Researchers have explored the development and testing of optical mining techniques for extracting water and volatiles from carbonaceous asteroids, particularly focusing on simulants called Nectar A and Nectar B. The study was published in *Acta Astronautica*. Recognizing asteroids as vital resources for space exploration and industry, the study aims to demonstrate how focused solar energy can induce thermal spalling—a process where brittle materials explosively fracture due to high thermal gradients—facilitating efficient resource extraction.

Image Credit: buradaki/Shutterstock.com

Background

Asteroids, particularly carbonaceous types, are rich in hydrated minerals capable of releasing significant quantities of water when heated. These resources are crucial for supporting long-

duration human missions and future space economies.

Thermal spallation, which forms the core of optical mining, involves heating the asteroid surface with concentrated solar energy, generating surface stresses that cause the brittle material to fracture and fragment.

Previous studies have examined the mechanics of thermal spallation in terrestrial contexts, notably in concrete technology, where factors such as thermal gradients, mineral composition, and pore pressure buildup influence failure behavior.

The unique environment of space and low-gravity conditions poses additional challenges and opportunities for mining operations. Understanding how mineral morphology affects fracture behavior, and beam parameters, particularly irradiance distribution, influence excavation rates, is essential for optimizing mining efficiency.

The Current Study

The authors utilized a dedicated optical mining testbed housed within a vacuum chamber that simulates space conditions. The chamber, equipped with precision measurement tools, including beam irradiance sensors, load cells for mass measurement, and residual gas analyzers (RGAs), allowed for real-time assessment of the mining process. They employed a high-powered laser system with adjustable beam properties to irradiate the simulant samples.

The simulants, Nectar A and Nectar B, differ primarily in their mineral content; Nectar B contains exfoliated vermiculite, which impacts its response to heating. The experimental procedure involved directing focused laser beams onto asteroid simulants to induce thermal spallation, while varied parameters such as beam irradiance levels and beam distribution profiles were systematically tested.

The team measured excavation rates, water vapor production, and mineral morphology changes. Post-test analyses included thermogravimetric analysis coupled with mass spectrometry (TGA-MS), enabling quantification of water and other volatiles released during the process.

Results and Discussion

Precise control over beam irradiance is pivotal for optimizing excavation rates. Variations in

irradiance distribution, especially over the laser's initial propagation distance in the vacuum chamber, significantly affected the spallation efficiency.

A higher irradiance beyond 350 W/cm^2 correlated with a decline in excavation performance, likely due to excessive localized heating leading to undesirable ductile behavior instead of brittle fracturing. This emphasizes the importance of maintaining optimal irradiance levels and beam uniformity for effective resource extraction. The experiments revealed a clear relationship between irradiance, mineral morphology, and volatile release: water and other volatiles were released more efficiently when the mineral structure remained brittle during heating.

The study also observed a characteristic "V"-shaped mining pattern, which resulted from uneven irradiance—center regions with higher intensity experienced faster excavation compared to the edges. Broader beam profiles with more uniform irradiance mitigated this pattern, leading to more consistent and predictable excavation outcomes. The addition of exfoliated vermiculite in Nectar B reduced the maximum achievable excavation rate compared to Nectar A and attributed to differences in mineral structure and mechanical response to thermal stress.

Thermogravimetric analysis showed that water release closely aligned with the heating profile, with peak water vapor emissions corresponding to temperature regimes where hydration minerals decompose. The study indicated that optimal water production occurred at specific irradiance thresholds, validating the importance of beam control strategies.

The research suggests that the brittle-to-ductile transition—a phenomenon where materials shift from brittle fracture to plastic deformation—plays a critical role in the efficiency of thermal spallation. Excessive heating or high irradiance can push minerals beyond the brittle regime, decreasing fragmentation and water release, and potentially damaging equipment or reducing resource yield.

Conclusion

The research advances the understanding of optical mining for asteroid resource extraction by demonstrating the critical influence of beam irradiance control and mineral morphology on excavation and volatile release rates. Precisely managed laser irradiation enables efficient thermal spalling while preventing the transition to ductile deformation modes that diminish fracture and water release. The study confirms that broader, more uniform beam profiles produce more consistent excavation patterns, which are crucial for scalable asteroid mining

operations.

The presence of exfoliated vermiculite in simulants reduces maximal excavation rates, indicating mineral composition's importance in process optimization. The results affirm that maintaining optimal irradiance—around levels that induce brittle fracture without surpassing the brittle-to-ductile transition—is key to maximizing resource extraction efficiency. These findings suggest that future in-space mining systems will benefit from advanced optical control, adaptive beam shaping, and thorough mineralogical assessments.

Journal Reference

Broslav T., Dreyer C., *et al.* (2025). Optical mining of carbonaceous chondrite simulants: Testing and lessons learned in asteroid mining research. *Acta Astronautica*, 235, 1–16. DOI: 10.1016/j.actaastro.2025.04.033, https://www.sciencedirect.com/science/article/pii/S0094576525002334?via%3Dihub

How Ion Mobility–HRMS Takes PFAS Detection Beyond Regulatory Limits

The US EPA has cataloged 14,735 PFAS species as manufactured compounds, precursors, and degradation products.[1] This makes their systematic and thorough monitoring particularly challenging. This study presents an innovative, non-targeted, suspect methodology for a comprehensive PFAS analysis, integrating trapped ion mobility spectrometry (TIMS) with LC-HRMS/MS data.

PFAS: Persistent Threats to Health and Environment

Per- and polyfluoroalkyl substances (PFAS) have become prominent environmental and public health concerns. Defined by the OECD in 2020 as *"fluorinated substances that contain at least one fully fluorinated methyl or methylene carbon atom (without any H/Cl/Br/I atom attached to it)"*, PFAS have been produced and utilized since the 1940s. Due to their resistance to heat, water, and grease, these substances have played essential roles in everyday products.

PFAS are often referred to as "forever chemicals" because of their persistent, bioaccumulative, and toxic (PBT) characteristics, as well as their widespread presence in the environment and living organisms.

While the associated health risks are not entirely understood for all PFAS, available evidence indicates that exposure may adversely affect reproduction and development, liver, kidneys, and the immune system, and may contribute to tumor formation.

Contamination by PFAS is now commonly observed in surface and groundwater, originating from sources such as landfills, agrochemical usage, industrial processes, firefighting operations, and other activities.

Regulating PFAS: Detection and Evolving Limits

PFAS is routinely quantified through liquid chromatography (HPLC) coupled to triple quadrupole (TQ) mass spectrometers. Multiple regulations and legal thresholds for PFAS concentrations were introduced in recent years, and these limits continue to evolve.

The US EPA has released the final National Primary Drinking Water Regulation (NPDWR) covering six PFAS compounds. Health advisories are currently in place for these compounds: PFOA and PFOS (4 ng/L interim), PFHxS, PFNA, and HFPO-DA (10 ng/L interim). The EU

Drinking Water Directive 2020/2184 includes a requirement to satisfy a limit of 100 ng/L for a list of 20 different PFAS or 500 ng/L for all PFAS.

Challenges in Comprehensive PFAS Monitoring

In 2023, five national authorities within the European Union (Germany, Denmark, the Netherlands, Norway, and Sweden) submitted a proposal for the total restriction on the production, marketing, and use of PFAS. Monitoring this restriction means the requirement for the detection and identification of the entity of all PFAS, extending well beyond the scope of current regulatory frameworks.

The US EPA estimates nearly 15,000 species in this group as manufactured compounds, precursors, and degradation products. This complicates their systematic and comprehensive monitoring. Due to the large number of PFAS compounds, only a limited fraction is accessible via reference standards or spectral databases, with many existing as isomers.

Consequently, conventional targeted analysis using TQ or high-resolution mass spectrometry (HRMS) encounters significant difficulties in achieving full coverage of this extensive chemical group. In response to the limited availability of standards and references, multiple initiatives have been established to compile PFAS data into suspect lists. The NORMAN network and NIST have developed suspect lists containing nearly 5,000 PFAS records.[2,3,4]

Novel Non-Targeted Approach for Comprehensive PFAS Analysis

A new non-targeted strategy is proposed for acquiring a holistic overview of PFAS, incorporating trapped ion mobility spectrometry (TIMS) with the mass spectral information from UHPLC-HRMS. The data is screened against traditional libraries and the suspect lists from NIST and NORMAN, enabling identification without needing reference libraries. This approach demonstrates enhanced performance over conventional methods with respect to time, reliability, and efficacy.

Methods

Sampling and Sample Preparation

Wastewater and surface water samples were obtained from 30 distinct locations across the Netherlands, representing various infrastructures such as industrial zones, urban areas, and natural or recreational regions. Solid-phase extraction was employed for sample purification and pre-concentration. Sample preparation followed the EPA 1633 regulation.

Samples were pre-concentrated by SPE using 25 mL of effluent from 200 mL of water. 50 µL of internal standards (IS) were introduced to the samples and the blanks. 4 mL 0.1% NH_4 OH buffer in MeOH was used for conditioning, and 4 mL 0.1% NH_4 OH in MeOH for elution and reconstitution. This yielded a 2,000-fold pre-concentration for surface water and 500-fold pre-concentration for effluents.

Analytical Workflow and PFAS Identification

2 µL of sample was injected into the LC/HRMS for a 20 min run time in negative ion mode. The MS method was optimized for PFAS with a parallel accumulation serial fragmentation (PASEF) acquisition workflow for non-targeted analysis for the suspect list screening.

The Elute UHPLC was equipped with a kit (Bruker) to remove PFAS originating from the tool. This system was coupled to the timsTOF Pro 2 (Bruker) with a high-sensitivity VIP-HESI (Vacuum Insulated Probe-Heated Electrospray Ionization) source. MS and MS/MS analyses were conducted in triplicate for each sample. Figure 1 outlines the analysis workflow. Following data acquisition and feature extraction, spectral library searches were performed in NIST and Bruker PFAS libraries.

Subsequently, the data was screened against the NORMAN network and NIST suspect lists. These lists contain basic information about the name, elemental composition, and InChI structure of almost 5,000 PFAS. Finally, unlisted compounds were identified using various MetaboScape® software (Bruker) instruments.

The MetaboScape software supports the ID Steps 2 and 3 using the following instruments:

- **SmartFormula** generates a list of potential elemental compositions for each compound.
- **CompoundCrawler** searches for corresponding structures for the proposed elemental compositions in databases and suspect lists.
- **MetFrag** applies comprehensive in-silico fragmentation using the structural information from InChI structures in the suspect lists or publicly available databases.[5]
- **CCS-Predict Pro** confirms the structure by comparing experimental CCS values and those predicted using the structural information from InChI structures in the suspect lists or from publicly available databases. Machine learning algorithms are employed to ensure high precision in CCS value prediction.[6]

Kendrick Mass Defect (KMD) Analysis for PFAS Detection

Filtration and reduction of specific features by Kendrick Mass Defect (KMD) plots is a popular

method for detecting and identifying chemically related compounds based on their exact mass. KMD evaluation filters potential PFAS from the matrix background, based on the CF_2 repeating units. KMD serves as a fundamental component of MetaboScape.

The Kendrick mass scale defines the mass of the recurring CF_2 unit in PFAS with a nominal value of 50 Da. The KMD is derived from the exact mass decimals of the end group of the respective PFAS sub-species. In a diagram, the KMD is plotted against the m/z scale. Homologous PFAS species with the same end group share identical KMD, aligning horizontally in the KMD plot with the addition of more CF_2 units. This enables differentiation from the remaining background signals.

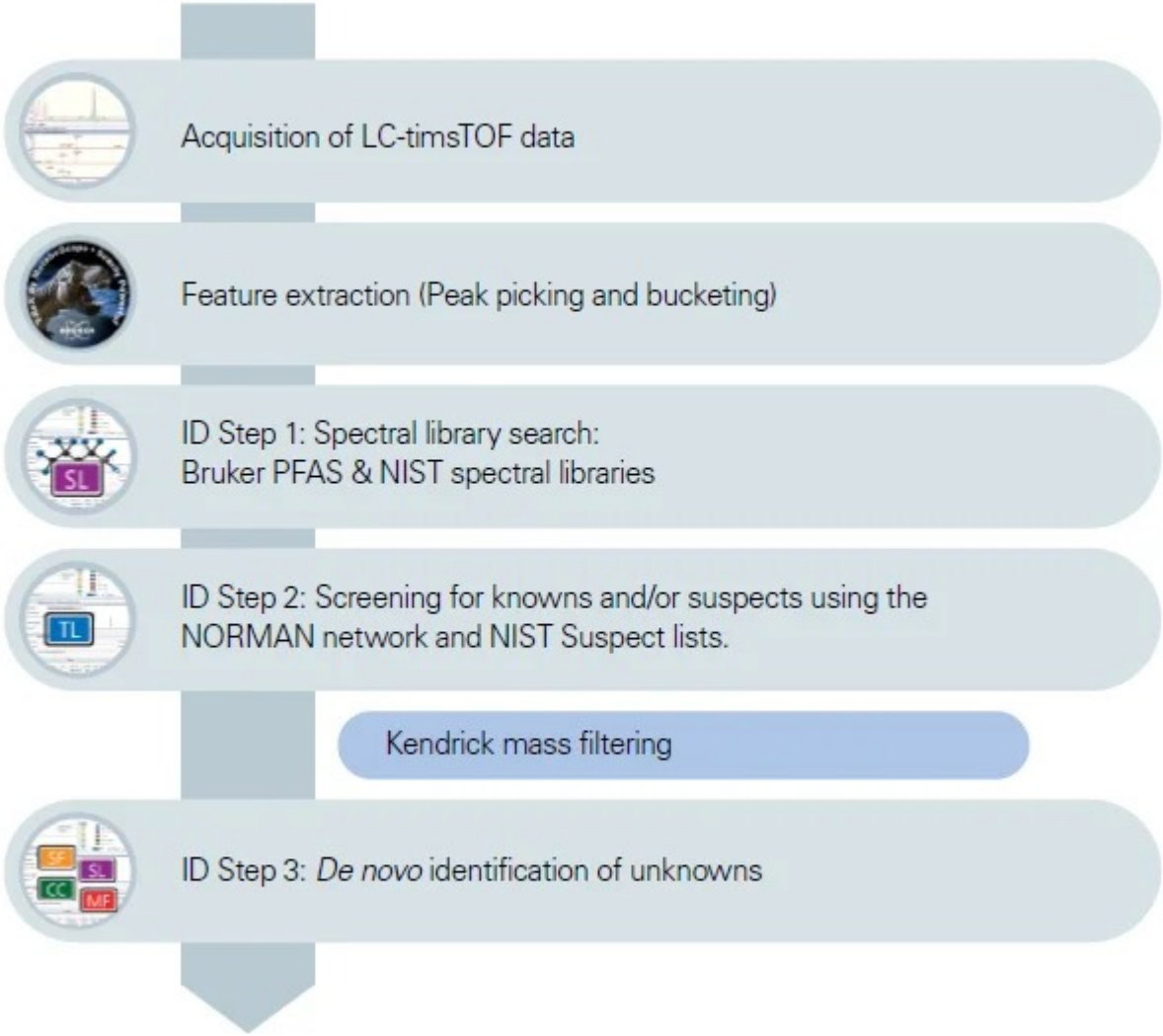


Figure 1. *Workflow of the data acquisition, data treatment and identification of the potential PFAS candidates; ID Step = Identification Step. Image Credit: Bruker Applied Mass Spectrometry*

Results

Utilizing TIMS for Enhanced PFAS Analysis

Recent approaches have applied high-resolution mass spectrometers (HRMS) to differentiate PFAS compounds through subtle differences in precise molecular weights and isotopic patterns. The primary challenge remains the low confidence in identifying many PFAS due to limited access to suitable, comprehensive libraries.

TIMS provides multiple ways to enhance performance when monitoring thousands of PFAS in a given sample. TIMS separates ions by their collisional cross sections (CCS), which are a function of shape and size. The ions are initially held stationary—or 'trapped'—by the two opposing forces of a pushing gas pressure and a repelling electrical field. By gradually reducing the electrical potential, each ion species is released in a controlled manner, with those of greater cross-sectional area eluting ahead of their more compact counterparts (Figure 2).

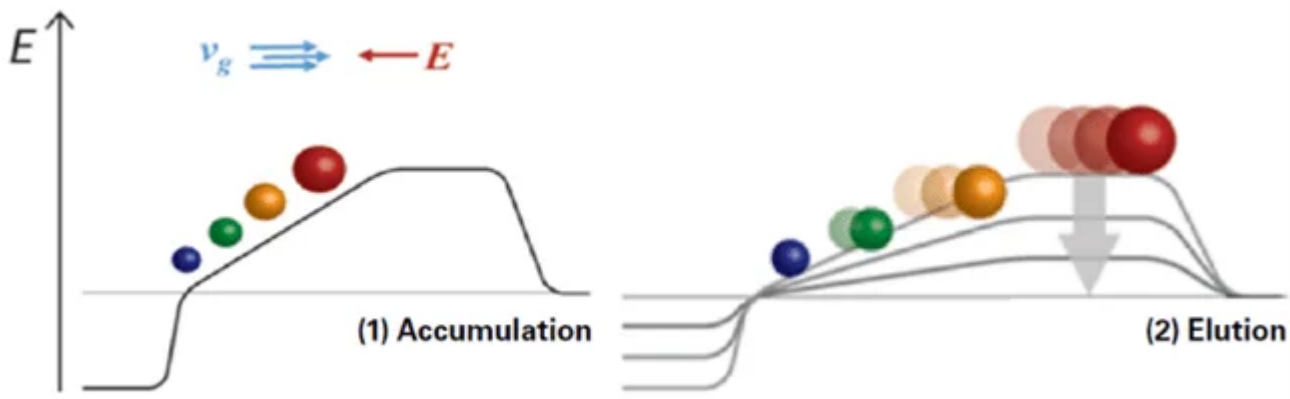


Figure 2. *TIMS principle based on the parallel accumulation/trapping and serial release of compounds based on their 3-dimensional structure and size. Image Credit: Bruker Applied Mass Spectrometry*

Collisional cross sections (CCS) thus serve as additional, orthogonal parameters to MS data, improving identification confidence. Additionally, TIMS ion trapping increases sensitivity and reduces PFAS detection limits via background elimination.

Lastly, it can be utilized to separate coeluting isobars and isomers, providing an additional separation to UHPLC-HRMS. This holds significant biochemical interest since physicochemical characteristics, such as those of linear and branched structures, may exhibit slight variance, leading to biochemical reaction and transformation differences,

bioaccumulation, and risk of toxic exposure.

Studies indicate that linear PFAS sorb preferentially to soil and sediments, while branched isomers are more likely to persist in water due to their increased polarity. Human serum samples can contain higher levels of branched PFOS compared to the ratio that is usually seen in the production of PFOS by electrochemical fluorination (70% linear).[7]

Enhanced Detection and MS/MS Coverage with PASEF

Figure 3 displays the heat map for a representative sample from ten different wastewater collection sites. The raw MS data exhibits over 8,600 detected features after extraction, underscoring the sample's complexity.

Since PASEF provides a considerably rapid MS/MS speed of >150 spectra/sec, MS/MS spectra cover 58% of all features. This uniquely high coverage is essential for ensuring the detection of compounds of interest, supporting comparison with in-silico fragments, and achieving final identification.

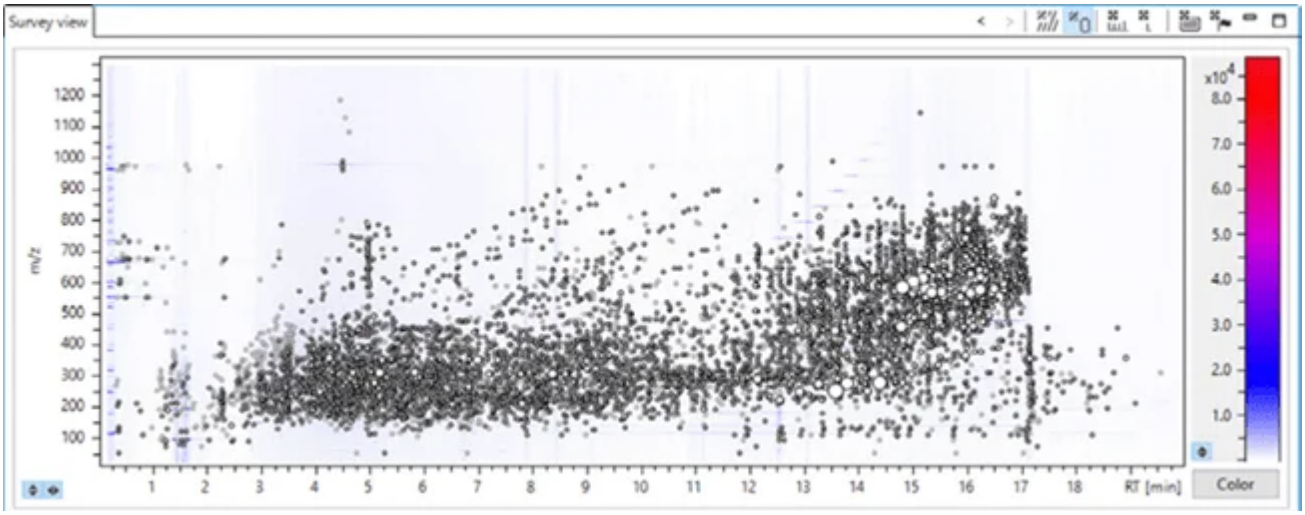


Figure 3. *Heat map for an effluent sample from The Netherlands. The retention time is plotted against the detected m/z with a color coding for the signal intensity. 8654 features have been detected after T-Rex processing (RT alignment of multiple features, recursive extraction of different ion species for the same compound). Image Credit: Bruker Applied Mass Spectrometry*

Simplifying Data Complexity with Kendrick Mass Defect

Kendrick mass defect (KMD) evaluation was employed in MetaboScape to filter PFAS signals from many other naturally occurring matrix compounds and reduce data complexity.

In this application, KMD filters potential PFAS from the matrix background based on the CF_2 repeating units. Candidates potentially related to PFAS appear as horizontal lines with discrete data points for the increasing CF_2 units along the m/z scale (Figure 4). The high mass accuracy the timsTOF Pro 2 provides is a key factor for efficient filtering.

Approximately 20,000 properties were detected from all effluents and surface water samples of the 30 sampling sites. After KMD filtering, approximately 500 potential PFAS candidates remained. This highly effective data reduction limits subsequent data analysis to relevant features only.

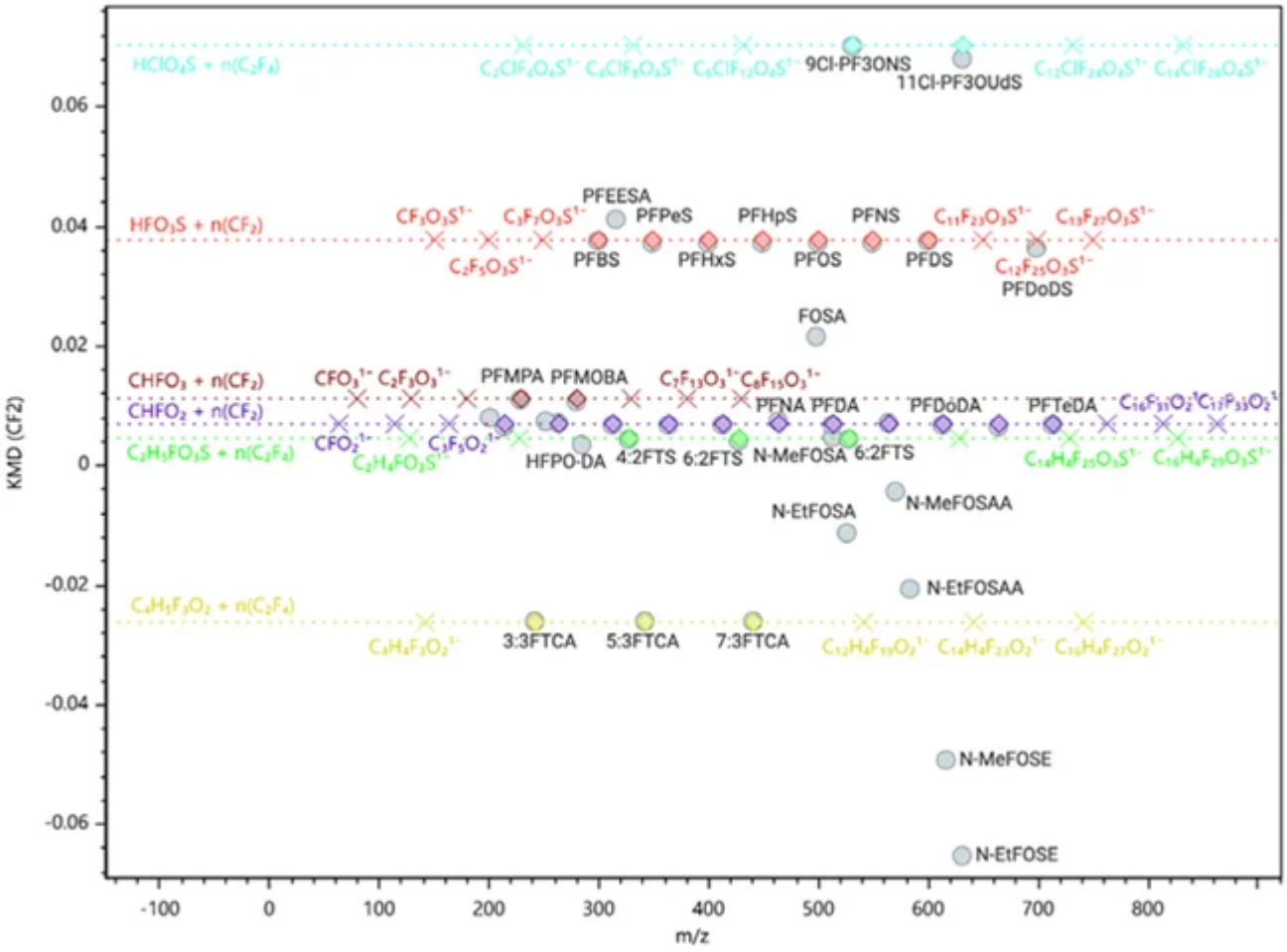


Figure 4. *Part of the KMD plot for a standard mixture according to the EPA Method 1633. PFAS of the same group are aligned in horizontal chains representing the addition of CF_2 units. MetaboScape supports the visualization and extension of these homologous rows. Image Credit: Bruker Applied Mass Spectrometry*

Multi-Criteria Approach for Confident PFAS Identification

Figure 5 presents a summary of results in MetaboScape, including an example of the experimental and library spectra match for a representative compound. For suspect list screening (ID Step 2) and de novo identification (ID Step 3), the combination of four different search criteria—exact mass, isotope pattern, MS/MS fragmentation and CCS value—was utilized.

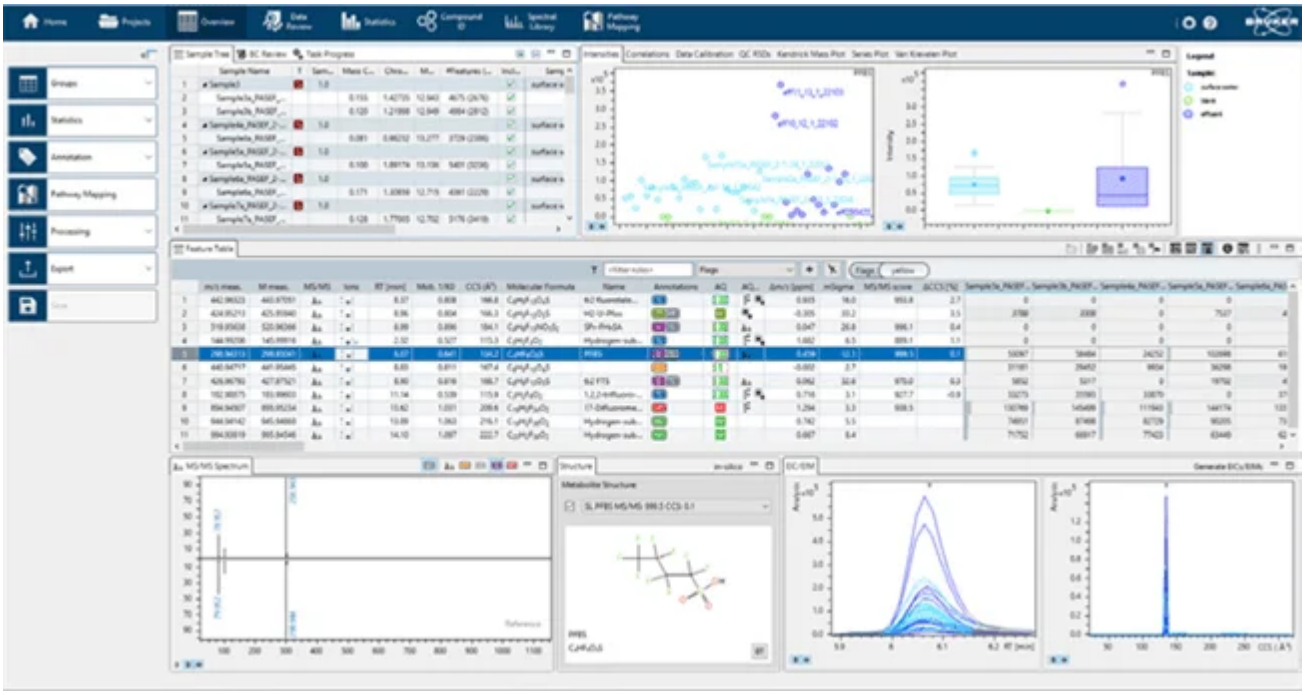


Figure 5. *Overview of the results in MetaboScape with a butterfly overlay of the experimental and the spectral data for a representative compound. Image Credit: Bruker Applied Mass Spectrometry*

The first two criteria were compared with the elemental compositions in the lists to generate a shortlist of candidates. The corresponding structures of these candidates from the suspect list (InChI) or public databases such as MetLin and PubMed were fragmented in silico by MetFrag and compared with the experimental MS/MS feature data.

Finally, experimental CCS (collisional cross section) values of remaining candidates were compared with machine learning-based predictions from the structures for the found suspects (CCS-Predict Pro). The combined match of these multiple orthogonal criteria generated a highly confident assignment of PFAS species without using reference standards.

Comprehensive PFAS Annotation in Wastewater

A total of 142 compounds in wastewater were annotated through a combination of steps: 12 were annotated via library search (ID Step 1, dark blue), 14 through the suspect lists (ID Step 2,

light blue), and 116 via de novo approach (ID Step 3) (Figure 6). This outcome emphasizes the necessity of utilizing high-information datasets, as numerous PFAS were detected that are absent from both libraries and suspect lists.

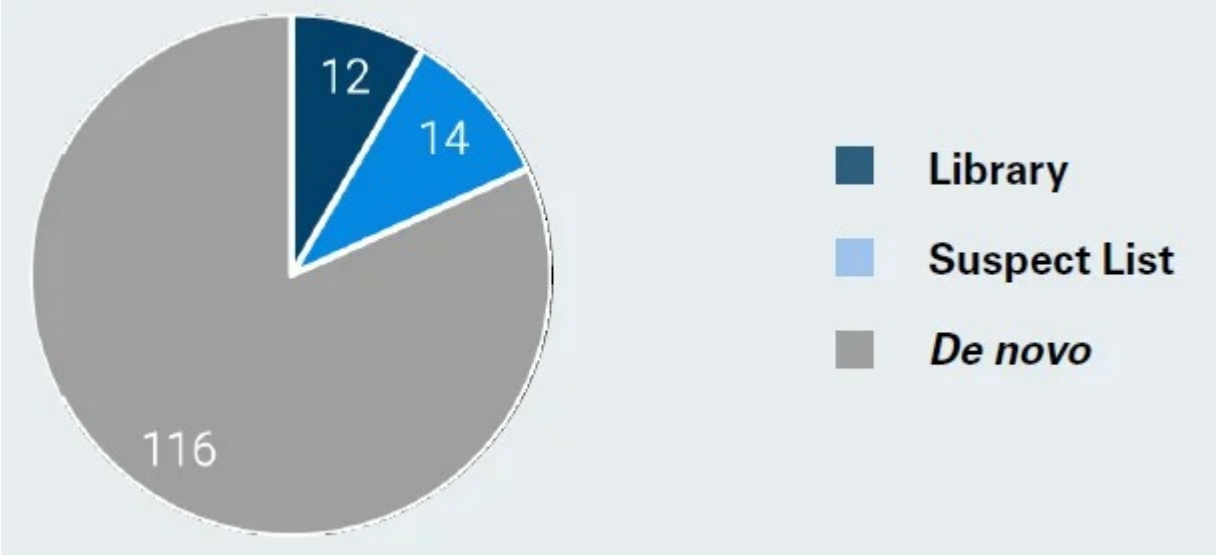


Figure 6. *The identification of 142 compounds in wastewater was achieved through various steps: 12 were annotated via library search (ID Step 1, dark blue), 14 through the suspect lists (ID Step 2, light blue), and 116 using the de novo approach (ID Step 3, grey). Image Credit: Bruker Applied Mass Spectrometry*

PFAS Distribution and Detection in Surface Water

In surface water samples, 137 features were annotated as PFAS. As expected from their local conditions and infrastructure, the quantity of detected PFAs varied among different sampling sites. Figure 7 compares these numbers across 18 sites.

Elevated contamination levels were observed at sites 1, 13 and 17, while lower contamination levels were visible at sites 4 and 15. Multiple PFAS precursors and degradation products were discovered that had not yet been screened in any legal directives and would have been missed in a targeted approach. In such cases, while targeted compounds would be quantified at low levels, the degradation products may exist at elevated levels, posing a potential hazard and health risks.

One example is H2-U-PFOS, identified in step 3. This unsaturated PFOS has previously been detected in the environment, although no commercial standard is currently available. Compounds of this type cannot be detected using existing target or library search methods.

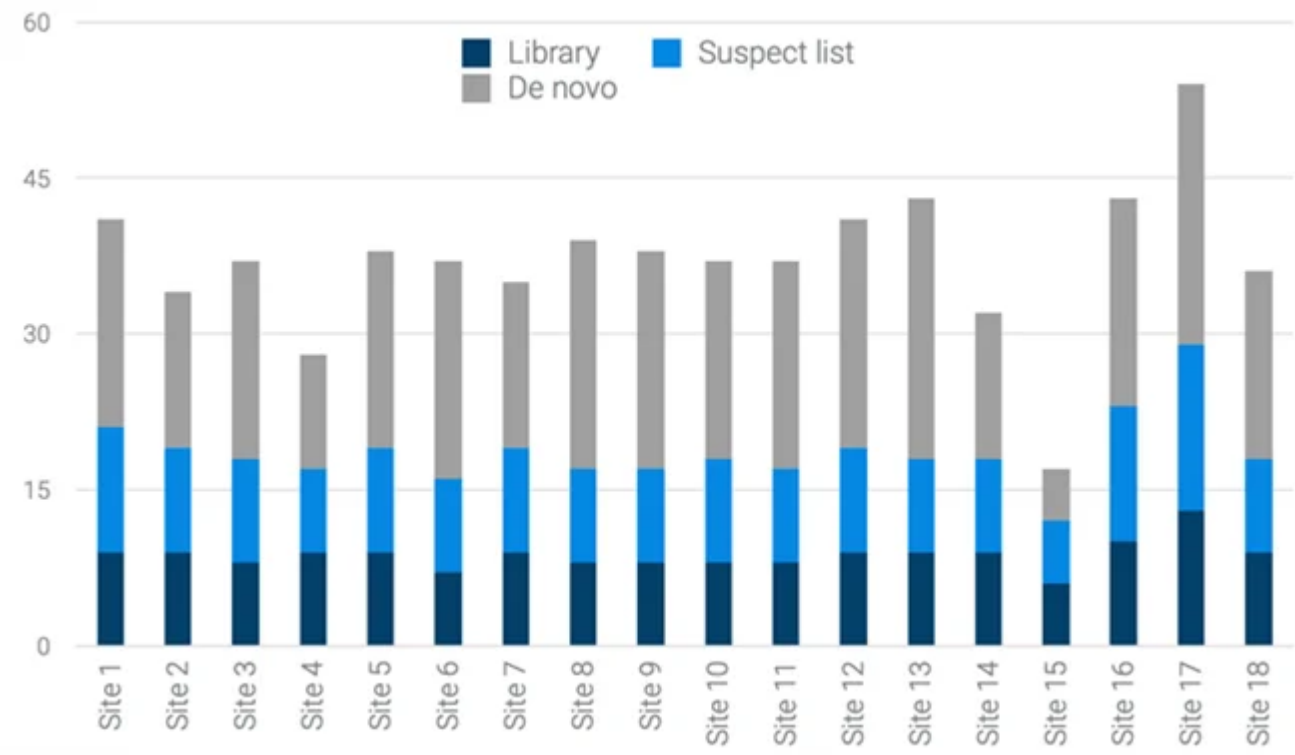


Figure 7. *Number of PFAS compounds found at the different surface water sites. While a higher number was observed e.g., at the sides 1, 13 and 17, lower contamination is visible e.g., at the sites 4 and 15. This is possibly due to the local infrastructure and environmental circumstances. Image Credit: Bruker Applied Mass Spectrometry*

Scoring Framework for Non-Target PFAS Analysis

The certainty of PFAS identifications based on HRMS data must be conveyed using a dependable and harmonized framework. Charbonnet et al. have recently proposed a confidence scale along with identification criteria tailored specifically for suspect or non-target analysis of PFAS by HRMS. Confidence levels range from 1a (Confirmed by Reference Standard) and 1b (Indistinguishable from Reference Standard) to 5 (Exact Masses of Interest).[8]

Incorporating structural data into the identification workflow by MS/MS and CCS values predominantly yields scoring levels of 1 and 2 (Table 1), thereby validating the reliability and high confidence of the combined Ion Mobility-HRMS methodology.

Additionally, the KMD filtering supports higher scores by annotating homologous compound series (level 2c). The study reinforces the necessity of non-target PFAS research and demonstrates the high sensitivity of the workflow in successfully identifying previously unknown or unanticipated PFAS products, precursors, and degradation compounds.

Table 1. Charbonnet scorings and respective results from the ion mobility-HRMS workflow presented here. The combination of mass accuracy, library search and structural information by MS/MS and CCS values results in scoring levels of 1 and 2. Source: Bruker Applied Mass Spectrometry

Level	Identification confidence	ID step
1a	Confirmed by reference standard	BDAL PFAS library including in-batch analysis of CRS
1b	Indistinguishable from reference standard	BDAL PFAS library
2a	Probable by library spectral match	NIST PFAS library
2b	Probable by diagnostic fragmentation evidence	Suspect list including *in-silico* fragmentation for MS/MS and CCS prediction
2c	Probable by diagnostic homologue evidence	Homologues PFAS series from KMD plots
3a	Positional isomer candidates	
3b	Fragmentation-based candidate	
3c	Circumstantial candidate with fragmentation evidence	
3d	Circumstantial candidate with homologue evidence	
4	Unequivocal molecular formula	
5a	PFAS suspect screening exact mass match	Just MS data comparison with suspect lists
5b	Nontarget PFAS exact mass of interest	

Conclusions

Addressing Analytical Challenges in PFAS Detection

Rigorous regulatory obligations increase the demand for robust and dependable PFAS detection and identification, yet the analytical difficulties remain considerable. Although thousands of PFAS exist, standards and libraries remain limited. Samples frequently contain compounds of interest in complex matrices.

Comprehensive 4D Workflow for PFAS Identification

This study outlines an innovative and unique strategy for matching high-quality 4D data of exact mass, isotope pattern, MS/MS, and CCS with data obtained from libraries and large

suspect lists. Utilization of the timsTOF Pro 2 and MetaboScape in combination with the "3 ID steps" indicates that all three annotation instruments were employed in sequential order to annotate one feature.

Library search, NIST or NORMAN network PFAS suspect list screening, and de novo compound elucidation proved an effective method for rapid and efficient identification of unknown PFAS in complex environmental matrices. It represents an intuitive workflow supported by automated feature finding and consecutive annotation, resulting in immediate results and data generation.

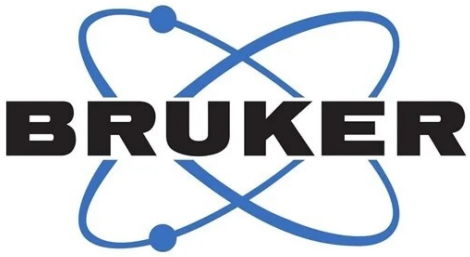
Advancing PFAS Analysis Beyond Targeted Methods

This method extends the PFAS analysis beyond the limitations of conventional targeted methodologies, allowing detection of a virtually limitless number of PFAS, including isomers in complex matrices. The strategy advances PFAS analysis to a level aligned with societal goals towards greater health and environmental protection and security for the future, beyond the scope of existing regulatory mandates.

References and Further Reading:

1. Computational Toxicology and Exposure Online Resources. *CompTox Chemicals Dashboard*. (online) Available at: https://comptox.epa.gov/dashboard/chemical-lists/PFASSTRUCT.
2. NORMAN. *NORMAN Substance Database*. (online) Available at: https://www.norman-network.com/nds/susdat/.
3. Benjamin Place (2021), Suspect List of Possible Per- and Polyfluoroalkyl Substances (PFAS),
4. National Institute of Standards and Technology, https://doi.org/10.18434/mds2-2387 (Accessed 2024-11-15)
5. Wolf, S., *et al*. (2010). In silico fragmentation for computer assisted identification of metabolite mass spectra. *BMC Bioinformatics*, 11(1). https://doi.org/10.1186/1471-2105-11-148.
6. Zhou, Z., *et al*. (2020). Ion mobility collision cross-section atlas for known and unknown metabolite annotation in untargeted metabolomics. *Nature Communications*, 11(1). https://doi.org/10.1038/s41467-020-18171-8.
7. Miralles-Marco, A. and Harrad, S. (2015). Perfluorooctane sulfonate: A review of human exposure, biomonitoring and the environmental forensics utility of its chirality and isomer distribution. *Environment International*, (online) 77, pp.148–159. https://doi.org/10.1016/j.envint.2015.02.002.

8. Charbonnet, J.A., *et al*. (2022). Communicating Confidence of Per- and Polyfluoroalkyl Substance Identification via High-Resolution Mass Spectrometry. 9(6), pp.473–481. https://doi.org/10.1021/acs.estlett.2c00206.



This information has been sourced, reviewed and adapted from materials provided by Bruker Applied Mass Spectrometry, developed in collaboration with Vrije Universiteit Amsterdam.

For more information on this source, please visit Bruker Applied Mass Spectrometry.

MassQL: A Universal Language for MS Data Analysis

In a recent *Nature Methods* article, researchers introduced MassQL, a universal language designed to change the way mass spectrometry (MS) data is queried and analyzed. The goal is to provide a standardized query language capable of capturing complex MS patterns, such as isotopic signatures, fragmentation spectra, retention times, and ion mobility details, in a format that is both consistent and computationally accessible.

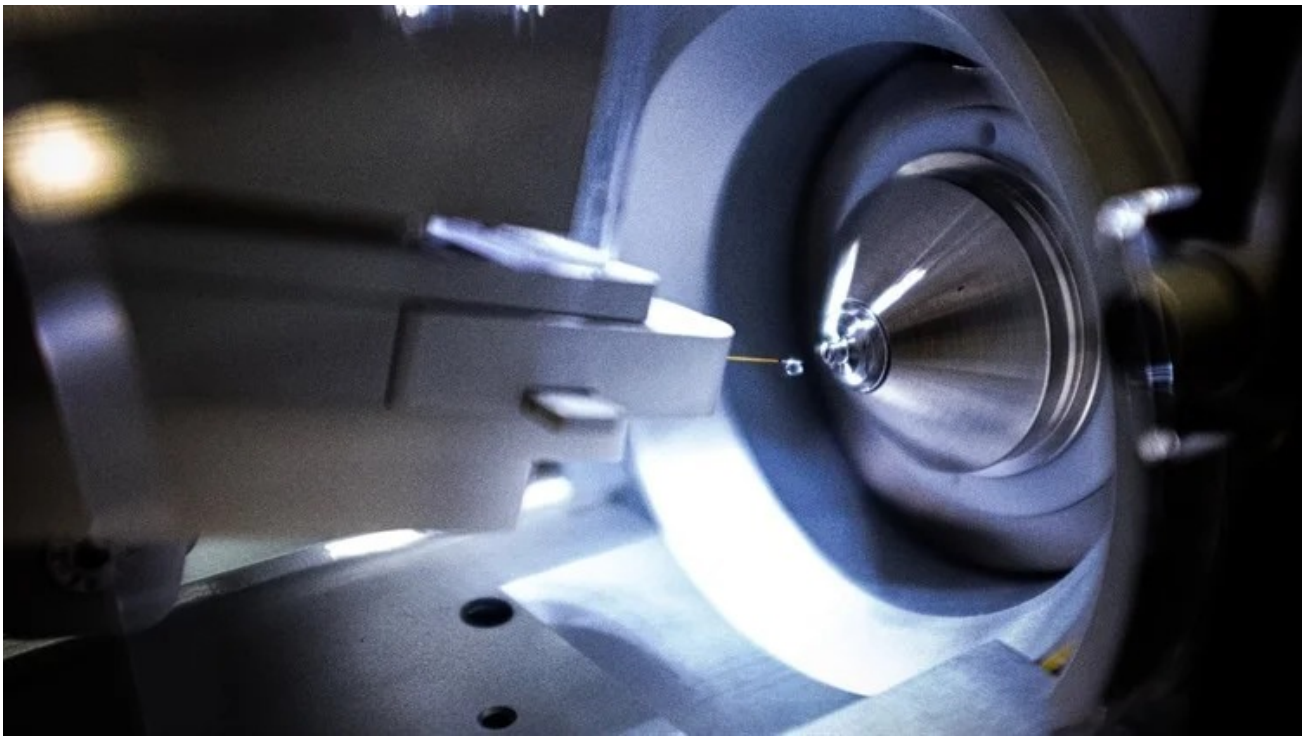


Image Credit: MSRG/Shutterstock.com

Background

Mass spectrometry operates much like an optical system: molecules are ionized, and their mass-to-charge ratios appear as spectral peaks. The complexity of MS data mirrors that of optical measurements, where patterns of light or spectral features reveal structural and compositional details. In MS, spectral patterns such as isotopic distributions, fragmentation residues, and retention times serve a similar role to optical signatures in spectroscopy and imaging, helping to identify and distinguish chemical entities.

Traditionally, data analysis tools have been tailored to narrow sets of patterns or designed for specific instruments, which limits the scope of analyte discovery. Manual inspection offers flexibility but is both error-prone and inefficient, especially with the growing scale of public

datasets. Existing analytical approaches (such as spectral library searches and similarity-based algorithms) work well in focused applications but struggle when tasked with uncovering unknown or structurally diverse molecules. This underscores the need for a flexible, formalized language for querying MS data, comparable to the way optical spectral analysis is used. Such a system would enable broader, more nuanced, and reproducible investigations across the field.

The Current Study

The development of MassQL centers on creating a formal grammar that defines how MS patterns can be expressed in a standardized syntax. Its technical architecture is designed to be instrument-agnostic, accommodating the wide range of ways MS data are generated and analyzed. The language supports queries on both MS1 (precursor ion) and MS/MS (fragmentation spectrum) data, covering features such as isotopic patterns, adducts, neutral losses, and fragment ions. It also integrates chromatographic and ion mobility constraints, enabling multidimensional pattern recognition.

A major strength of this approach lies in its extensibility. The grammar set is structured for community-driven growth, making it possible to incorporate new terms and features seamlessly. The implementation is built on open-source components, including parsers and an engine that can run independently or within software platforms such as MS-DIAL, Mzmine, and Bruker's MetaboScape. This adaptability resembles optical systems that can be calibrated or adjusted for different imaging setups.

Equally important is the validation of MassQL through real-world applications. The authors highlight its ability to handle large datasets from public repositories such as GNPS/MassIVE, Metabolomics Workbench, and MetaboLights. By applying mass accuracy, intensity thresholds, and Boolean logic, they construct precise queries similar to optical filters that selectively pass or block certain spectral features. This allows for detailed pattern detection on a large scale.

Results and Discussion

The application of MassQL delivers promising results, showing its ability to scan large MS datasets for predefined patterns with both specificity and flexibility. The authors provide examples where the tool successfully identifies molecules based on distinct spectral features such as characteristic fragment ions or neutral losses, which serve as hallmark signatures in MS much like spectral lines in optical spectroscopy. This capability supports targeted discovery of chemical compounds, including structurally related analogs and molecules with subtle modifications that might be missed by traditional similarity searches.

A key advantage of MassQL is its flexibility in combining different types of MS data, including retention time, isotopic patterns, and fragmentation spectra. When paired with Boolean operators, these elements enable more refined and multidimensional searches. This further strengthens the analogy to optical spectroscopy, where integrating multiple wavelengths or spectral features produces deeper insight into the composition of a target analyte.

The study also highlights MassQL's use as a pre-filtering tool ahead of more resource-intensive methods such as spectral library matching or molecular networking. The authors quantify false discovery rates and acknowledge that some false positives are unavoidable, yet demonstrate how the strategic integration of MassQL queries with downstream validation significantly improves confidence in results. This approach is comparable to optical systems, where filtering and subsequent validation are critical for accurately interpreting complex spectra or images.

From an analytical standpoint, the software embodies principles of optical pattern recognition and information filtering, translating intricate spectral data into a formal language that enables reproducible, large-scale searches.

Conclusion

The study presents MassQL as a platform-independent and flexible query language that broadens access to complex MS datasets, allowing researchers to explore molecular signatures without requiring extensive computational expertise. Its design reflects the principles of optical pattern recognition and spectral analysis, where high-dimensional data are interpreted through established signatures. By framing MS data within a linguistic structure, the authors introduce a framework that strengthens reproducibility, fosters interoperability, and expands opportunities for discovery on a large scale. In practice, MassQL has the potential to reshape how scientists interrogate the molecular universe, making the depth of MS data more accessible and interpretable in much the same way that advances in optics have enriched our understanding of light and matter.

Journal Reference

Damiani T., Jarmusch A.K., et al. (2025). A universal language for finding mass spectrometry data patterns. *Nature Methods* 22, 1247–1254. DOI: 10.1038/s41592-025-02660-z, https://www.nature.com/articles/s41592-025-02660-z

Next-Generation Mass Spectrometry Coupled with Microfluidics for Trace-Level Hazmat Analysis

Trace-level hazardous materials (Hazmat) analysis involves monitoring, identifying, and quantifying minute concentrations of harmful substances, such as toxic chemicals, volatile and semi-volatile organic compounds (VOCs), microbes, and heavy metals, to protect humans and the environment.

Image credit: JU.STOCKER/Shutterstock.com

Numerous organic and inorganic substances are introduced into the environment through various human activities, including deforestation, pollution, industrialization, and chemical spills. The current article focuses on the benefits of next-generation mass spectrometry (MS) coupled with microfluidics for trace-level Hazmat analysis.

Conventional Technique for Trace-Level Hazmat Analysis

Traditionally, scientists have used spectroscopic, electromagnetic, and chromatographic techniques to detect various materials. Several conventional methods have shown low specificity, long analysis times, and limited sensitivity in detecting trace quantities.[1]

Spectroscopic methods, such as atomic absorption spectroscopy (AAS) and inductively coupled plasma-mass spectrometry (ICP-MS), are typically employed to detect and quantify metals. In contrast, chromatographic methods (e.g., gas chromatography, GC, and liquid chromatography, LC) are used to analyze organic compounds. Often, scientists combine two approaches to enhance detection accuracy.

Each technique comes with its benefits and limitations. For instance, many conventional methods generate false positives due to background radiation, temperature fluctuations, and humidity variations. Additionally, instruments for these techniques, such as GC-MS and ion mobility spectrometry (IMS), are bulky and slow. Thermal imaging is also used for trace-level Hazmat analysis; however, this method is limited by evaporation rates and surface properties.

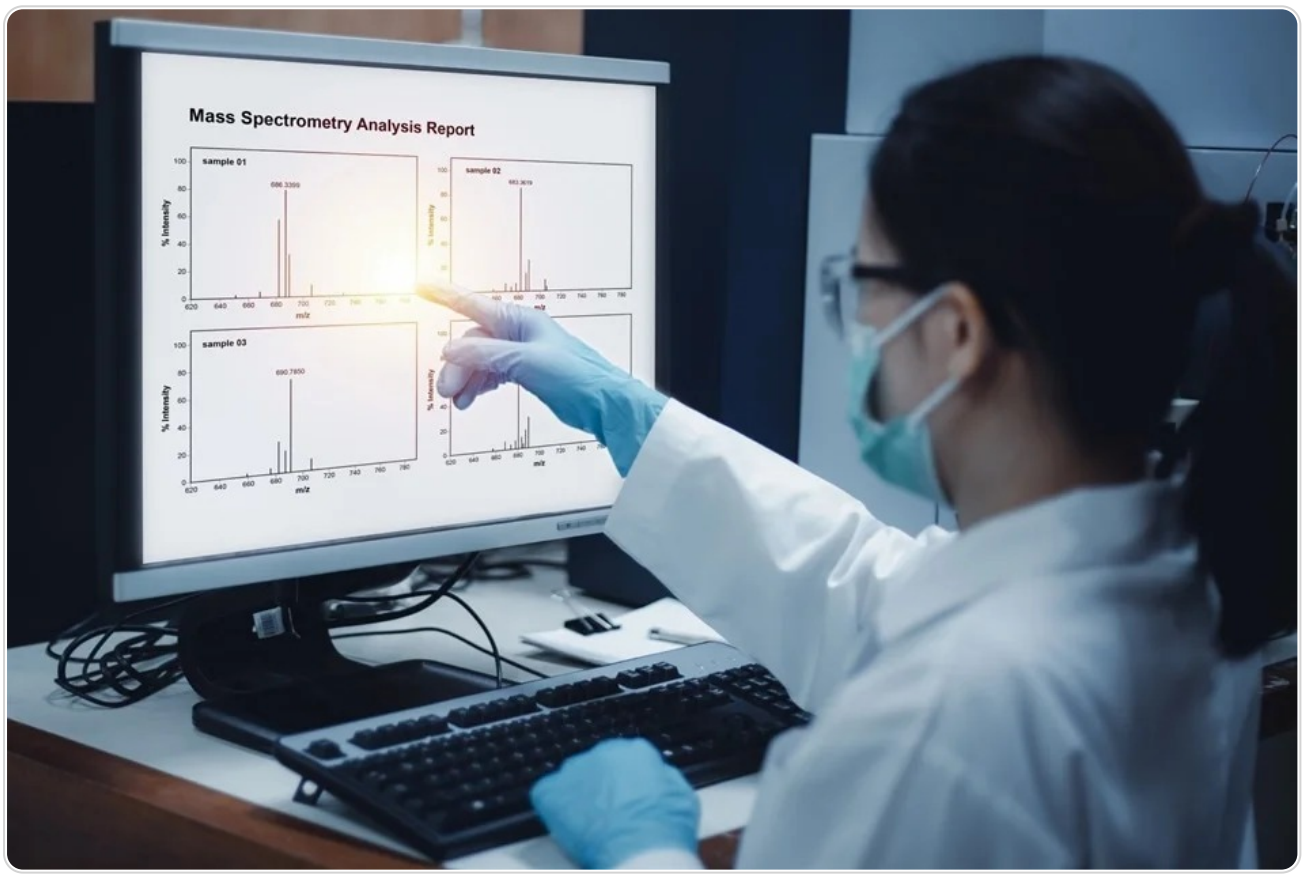


Image credit: S. Singha/Shutterstock.com

MS Coupled With Microfluidics Devices to Detect Trace Elements

Compared to benchtop instruments, microfluidic device miniaturization offers great benefits in chemical analysis. Besides miniaturization, which promotes reduced use of analytical reagents, microfluidic devices can integrate multiple analytical processes on a single platform, ensuring higher assay sensitivity.[2] This approach offers parallel analysis domains for automated and high-throughput assays that significantly reduce errors frequently generated

from manual sample handling.

Microfluidic devices are integrated with MS through electrospray ionization (ESI).[3] Scientists have coupled MS to microfluidic systems to minimize sample and reagent volumes, increase analysis speed, enhance sensitivity, and enable both quantitative and qualitative analysis.

Droplet microfluidic (DMF) systems use an inert carrier fluid to compartmentalize reactants and encapsulate aqueous samples in droplets.[4] This method generates droplets with volumes ranging from 0.05 pL to 1 nL, which can encapsulate DNA, cells, or other molecules within the aqueous phase while minimizing the risk of cross-contamination. Although theoretical maximums have been reported, DMF systems can screen up to 108 samples in practice in one day. By coupling MS with DMF, scientists can perform high-throughput screening applications.

A microfluidic chip-based multi-channel ionization (MCMCI) system has been developed to extract untreated compounds from complex matrices for trace element analysis using MS.[5] The microfluidic chip integrates ionization into a miniaturized format, improving processing speed and accuracy.

A microfluidic platform coupled with various detection systems, including MS, supported by high-speed computation and an artificial intelligence (AI) network, significantly accelerates identifying and quantifying pollutants in water and soil samples.[6] This approach shortens detection time and increases detection efficiency. Combining AI with a microfluidic device has proved to be a powerful tool for predicting heavy metal pollution.

Applications Of Microfluidic-MS Devices for Trace Element Analysis

Uranium And Actinide Separation

A novel microfluidic-MS device has been developed to directly analyze trace elements and uranium directly, minimizing operator-sample interaction.[7] This device can separate uranium from key trace elements using nitric acid solutions of different concentrations and chromatographic resins for adsorption and recovery. The eluates from this microdevice are diluted and directed to an ICP-MS system for radiochemical analysis. This highly sensitive strategy also lowers the cost of trace elemental analysis.

Biomedical Monitoring of Toxic Metals

Analysis of trace elements is crucial to monitoring the physiological environment. By coupling a microfluidic chip with ICP-MS, researchers enabled the detection of gadolinium in human body fluids.[8] Gadolinium is a naturally occurring rare earth metal, which is extremely toxic in its free elemental form. Although it is commonly used in MRI scans to enhance image clarity

and is considered safe, it may lead to severe kidney dysfunction.

Heavy Metal Detection in Biological Samples

A titanium dioxide-assisted preconcentration/*on-site* vapor generation chip, coupled with ICP-MS, was developed to detect mercuric ions in urine samples.[9] Furthermore, three three-dimensional microfluidic devices coupled with ICP-MS have also been designed to detect cadmium, mercury, and lead in a single cell. Long-term exposure to heavy metals may result in neurological problems, including cognitive impairment, memory loss, diminished motor skills, behavioral changes, and kidney dysfunction.

Food Safety and Microbial Detection

Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry MALDI-MS is a powerful analytical instrument to determine proteins, peptides, and nucleic acids. An automated microfluidic chip coupled with MALDI-MS has been developed to detect spoilage microorganisms in the food industry rapidly.[8]

Chemical Warfare Agents

Using a magnetic bead-based solid-phase extraction, a digital microfluidic device (DMF) extracts and purifies the chemical, and the resultant solution is loaded onto a MALDI plate to determine the chemical warfare agent stimulant.[10]

AI-Enhanced Environmental Monitoring

Integrating AI and machine learning in microfluidic devices has significantly enhanced water quality monitoring systems. Scientists have designed a portable, microfluidic-based biosensor to detect mercury in seawater's nanomolar (nM) range.

A machine learning algorithm was developed to analyze fluorescence data generated by a microfluidic device. The dataset was compiled and categorized using actual fluorescence values to predict mercury concentration. This approach enables personnel to monitor on-site marine pollution without specialized training.[6]

Emerging Trends in Multi-Parameter Detection

Currently, scientists are focusing on developing more sophisticated algorithms for microfluidic chip data analysis to enhance the accuracy of contaminant detection. A more advanced multi-parameter detection device equipped with intelligent data analysis will aid in the early detection of trace elements, thereby preventing harmful effects on humans and the environment.

Video credit:bostonuniversity/Youtube.com

Validation, Regulatory, And Operational Limitations

Despite promising technical advances, several challenges remain before microfluidic-MS devices can be widely deployed for Hazmat detection. Validation of new devices against standardized reference materials is essential to ensure reproducibility and comparability across laboratories. Regulatory approval processes can be lengthy, particularly for systems intended for clinical or defense use, where biosafety and data security requirements are stringent.

Operational limitations also exist. Portable microfluidic-MS systems must be sturdy for field environments and capable of handling variable humidity, temperature, and dust exposure without performance loss. Furthermore, routine calibration and maintenance can limit deployment in resource-limited or emergency-response settings. Addressing these constraints will be critical to translating laboratory innovations into reliable field applications.

Future Outlooks

Looking ahead, integrating microfluidic-MS platforms with cloud-connected data systems and remote AI analysis could enable real-time global monitoring of environmental hazards.

Advances in additive manufacturing may reduce device costs and enable rapid customization for specific threat profiles, from industrial contaminants to chemical warfare agents.

Furthermore, a greater focus on interoperability with existing emergency response infrastructure, such as handheld detectors and mobile labs, will enhance operational impact.

While significant work remains, combining microfluidics, next-generation MS, and machine learning has the potential to transform trace-level Hazmat analysis into a faster, more accurate, and more field-deployable technology.

References

1. Li Y, et al. Advances in environmental pollutant detection techniques: Enhancing public health monitoring and risk assessment. *Environ Int*. 2025;197, 109365. doi.org/10.1016/j.envint.2025.109365
2. Das A, Prajapati P. Navigating pharmaceuticals: microfluidic devices in analytical and formulation sciences. *Discov Chem.* 2025; 2, 49. doi.org/10.1007/s44371-025-00133-y
3. Wang X, et al. Microfluidics-to-mass spectrometry: a review of coupling methods and applications. *J Chromatogr A*. 2015;1382:98-116. doi: 10.1016/j.chroma.2014.10.039.
4. Ha NS, et al. Faster, better, and cheaper: harnessing microfluidics and mass spectrometry for biotechnology. *RSC Chem Biol*. 2021;2(5):1331-1351. doi: 10.1039/d1cb00112d.
5. Yu C, et al. Multi-channel microfluidic chip coupling with mass spectrometry for simultaneous electro-sprays and extraction. *Sci Rep*. 2017;7(1):17389. doi: 10.1038/s41598-017-17764-6.
6. Zhang Y, et al. Artificial Intelligence-Based Microfluidic Platform for Detecting Contaminants in Water: A Review. *Sensors (Basel)*. 2024;24(13):4350. doi: 10.3390/s24134350.
7. Han SY, et al. Development of an automated microfluidic system for actinide separation and analysis. *J Chromatogr A*. 2025;1742:465646. doi: 10.1016/j.chroma.2024.465646.
8. Chen J, et al. Integrated microfluidic chip coupled to mass spectrometry: A minireview of chip pretreatment methods and applications. *J Chromatogra Open*. 2021; 1, 100021. doi.org/10.1016/j.jcoa.2021.100021
9. Shih TT, et al. Development of a titanium dioxide-assisted preconcentration/on-site vapor-generation chip hyphenated with inductively coupled plasma-mass spectrometry for online determination of mercuric ions in urine samples. *Anal Chim Acta*. 2019;1063:82-90. doi: 10.1016/j.aca.2019.02.035.
10. Lee H, et al. Sample preparation of chemical warfare agent simulants on a digital microfluidic (DMF) device using magnetic bead-based solid-phase extraction. *Microfluid Nanofluid*. 2017;21, 141. doi.org/10.1007/s10404-017-1976-6