12th Nordic Conference on Plasma spectrochemistry and ionisation principles in mass spectrometry – From elements to molecules

June 14 - 18 2026, Loen, Norway

Programme and Abstracts

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2 Welcome Letter

On behalf of the Analytical Section of the Norwegian Chemical Society it is a great honour and pleasure to welcome you to Loen and to the *12th Nordic Conference on Plasma Spectrochemistry and Ionisation Principles in Mass Spectrometry - From Elements to Molecules*. With about 100 participants gathered, this meeting provides both an international and regional forum for sharing knowledge, debating ideas, and exploring the latest advances across the vibrant landscape of plasma-based analysis.

This year marks an important evolution reflected in our conference title. What began as a focus on elemental and isotopic analysis, has matured into a broader vision that embraces speciation analysis, metallomics, and the integrated determination of elemental and molecular information. From ionisation sources to spectrometer design, new instrumentation and the inventive adaptation of established systems now enable simultaneous or quasi-simultaneous measurement of atoms, molecules, and molecular fragments - even for transient samples emerging from chromatography, laser or ion ablation, and thermal volatilization. Our plenary lectures will trace this journey from past innovations to present capabilities and cast a forward-looking eye toward the devices and methods that lie ahead.

Central to our mission is cultivating a space where experience meets curiosity. We extend a particularly warm welcome to students and young scientists. Throughout the four-and-a-half-day programme, you will find short tutorial courses led by leading authorities designed to demystify theory, sharpen practical skills, and offer expert guidance for method improvement and novel applications. These tutorials, together with discussions, posters, and networking opportunities, are meant to accelerate your growth and amplify your voice within our community. We encourage senior researchers and industry practitioners to actively engage with our emerging colleagues - mentorship and dialogue are the lifeblood of sustained scientific progress.

Our plenary programme assembles some of the world's foremost experts to provide a comprehensive overview of recent developments in plasma spectrochemistry and ionisation principles in mass spectrometry. Yet the spirit of this meeting reaches beyond disciplinary boundaries. We hope you will use this week to spark collaborations across fields, cultures, and generations - bringing together fundamental insights, instrumental advances, and application-driven questions to create new possibilities.

There is something extraordinary about meeting in person. The collective energy of great minds in one place inspires fresh thinking and new partnerships. Loen's natural beauty offers a setting that both calms and invigorates; we hope it will frame your work with perspective and joy. May the excursions, social events, and outdoor farewell dinner complement the scientific endeavour and help forge lasting connections.

To first-time attendees: a special welcome. We are delighted that you are joining us, and we hope this conference becomes a milestone in your scientific journey. To our returning colleagues: thank you for continuing to shape and strengthen this community.

We wish you an engaging, productive, and memorable stay in Loen. May this week advance our shared pursuit - from elements to molecules - and illuminate the future of plasma spectrochemistry and mass spectrometric ionisation.

Warmly
The Organising Committee,

3 Organising and Scientific Committee

Yngvar Thomassen	(Conference Chair), National Institute of Occupational Health, Oslo and Norwegian University of Life Sciences, Ås, Norway
Balazs Berlinger	University of Veterinary Medicine, Budapest, Hungary
Estela Reinoso-Maset	Norwegian University of Life Sciences, Ås, Norway
Debora Foppiano	SINTEF, Trondheim, Norway
Ivar Martinsen	(Treasurer) Norwegian Chemical Society, Oslo, Norway
Arne Åsheim	(Exhibition Coordinator), Norwegian Chemical Society, Porsgrunn, Norway

4 General Information

Conference Desk

The conference desk is situated in the conference foyer of Hotel Alexandra. It will operate as follows:

Saturday	13 June	15:00 - 18:00
Sunday	14 June	08:00 - 09:00
Monday	15 June	07:30 - 08:00
Tuesday	16 June	07:30 - 08:00
Wednesday	17 June	07:30 - 08:00
Thursday	18 June	08:00 - 09:00

Participants are requested to register as soon as possible upon arrival to the conference venue, Hotel Alexandra, Loen.

Conference Venue

All oral and poster sessions will be held in the various auditoriums of Hotel Alexandra.

Tel: +47 57 87 50 00 Fax: +47 57 87 50 51 Email: alex@alexandra.no
Homepage: www.alexandra.no

Meals

Participants staying at Hotel Alexandra are served breakfast, lunch and dinner (all included in their accommodation package).

5 Social Programme

Saturday 13 June, 17:00 - 19:00 Informal get-together in the Hotel Alexandra Bath & Spa

All delegates and accompanying persons are invited to enjoy the heated outdoor swimming pool and refreshments.

Sunday 14 June, 14:00: Half-day excursion to Geiranger

This tour encompasses a mountain plateau above the tree and snow lines, the summit of Dalsnibba (1746 m), and a sail of 25 km along the spectacular Geirangerfjord.

Sunday 14 June, 14:30: Boat tour at Loen Lake

The MS Kjenndal II takes you on a trip from Sande at the lower end of the Loen Lake to Kjenndalsanden, where Kjenndalstova is located. A one-hour stop allows for a walk or you can enjoy delicious waffles and hot coffee before the boat returns to Sande.
The trip takes around 4 hours.

Sunday 14 June, 14:00: The Skåla Challenge

Those who want to challenge the Norwegian mountains after lunch may visit the Klaumann Tower at Skåla Mountain. This is the hardest uphill walk in entire Norway, approx. 1800 m straight up (8 km). Hikers are advised to bring appropriate footwear and clothing for this walk.
Free of charge, but you will sweat!

Sunday 14 June, 14:00: Loen Skylift

Loen Skylift is a spectacular attraction and adventure arena in the inner part of the Nordfjord. A cable car will lift you from the fjord to 1011 m above sea level. Here you can enjoy the views of the fjord landscape – from the restaurant table, or while exploring in the mountains.

Sunday 14 June, 14:00: Via Ferrata Loen

Via Ferrata Loen is a climbing path secured with wire right behind Hotel Alexandra. The climbing trail takes you to the top of Hoven at 1011 meters above sea level, with a phenomenal view of Loen and Olden Vally.
As part of the route you can cross Gjølmunn Bridge, the longest Via Ferrata bridge in Europe**.** The bridge is located 750 meters above sea level and is 120 meters long.

Monday 15 June, 21:00: Bring your own to the poster viewing beverage tasting

You are invited to bring your favourite beverage to be enjoyed by you and others!

Wednesday 17 June 16:10: Excursion to the Briksdal Glacier with a conference outdoor dinner

You are invited to visit the heart of Norway - an **Unforgettable** trip to the Briksdal Glacier. Participants can enjoy a walk to view the glacier arm and test the best aquavit in the world; *Gilde Aqua Ultra Plus*, or the local *Loen Apple Juice.*

Afterwards there will be the famous outdoor barbeque at "Kleivane" (weather permitting - otherwise the grill party will be held at Briksdalen Inn).
The well-known Norwegian gourmet chef Frode Aga will once again be in charge of the kitchen to ensure your best outdoor food experience.
This event is kindly sponsored by Shimadzu Europe and Massanalys Spectrometry Nordic.

6 Scientific Programme

Oral presentations
Invited plenary lectures and submitted oral contributions will be 30 and 20 minutes in length, respectively (including discussion).
Video projectors will be provided in all lecture rooms.

Posters
The posters should be mounted Saturday afternoon or early Sunday morning, in the poster area located next to the lecture room. Materials for poster mounting are available either from the conference desk or in the poster mounting area.

Language
The working language of the conference is English.

7 Liability

The Organising Committee declines any responsibility whatsoever for injuries or damages to persons or their property during the conference.

8 Sponsors and Exhibitors

The conference is sponsored by:

The Research Council of Norway

nu / AMETEK

SHIMADZU Excellence in Science

Amsnordic

MiMaC
Norwegian Laboratory for Mineral and Materials Characterisation

SPS Spectrapure Standards

NKS

The exhibition of scientific instrumentation, literature and consumables is located next to the auditorium at the first floor.

The following companies have registered for display and demonstration:

Elemental Scientific Nordics AB
Houm AS
Matriks AS/Agilent Technologies/Inorganic Ventures
Njbinglab
Nu Instruments Ametek
Shimadzu Europa GmbH
Thermo Fisher Scientific

9 Correspondence after the conference

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Vitesse

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10 Schedule of events

Saturday 13 June 2026

15:00 - 18:00	**Registration**
17:00 - 19:00	**Informal get-together in the Hotel Alexandra Bath & Spa** *This event is kindly sponsored by Spectrapure Standards AS*
From 19:00	**Dinner**

Sunday 14 June 2026

08:00 - 09:00	**Registration**
08:45 - 09:15	**Welcome and opening remarks**
09:15 - 11:15	**Session I: Frontiers in atomic and molecular spectrochemistry**
11:15 - 11:45	**Coffee break, poster viewing and exhibition**
11:45 - 12:45	**Session I continues: Frontiers in atomic and molecular spectrochemistry**
13:00 - 14:00	**Lunch**
14:00 -	**Excursion to Geiranger, The Skåla Challenge, Loen Skylift and Loen Lake**
From 19:00	**Dinner**

Monday 15 June 2026

08:00 - 10:10	**Session II: Progress in instrumentation and application of spectrochemistry**
10:10 - 10:40	**Coffee break, poster viewing and exhibition**
10:40 - 13:00	**Session III: Ionisation, laser ablation and elemental/molecular imaging**
13:00 - 14:00	**Lunch**
14:00 - 15:10	**Session III continues: Ionisation, laser ablation and elemental/molecular imaging**

Short Courses Session I

15:20 - 17:05	**Short course A1**	**Short course A2**	**Short course A3**	**Short course A4**	**Short course A5**
17:05 - 17:30	**Coffee break, exhibition and poster viewing**				

Short Courses Session II

17:30 -19:15	**Short course B1**	**Short course B2**	**Short course B3**	**Short course B4**	**Short course B5**
From 19:00	**Dinner**				
21:00	**BYOB gathering with exhibition, poster viewing and discussions (*remember to bring your drink of choice*)**				

Tuesday 16 June 2024

08:00 - 11:20	**Session IV: Molecular and biological mass spectrometry imaging**			
10:00 - 10:30	**Coffee break, poster viewing and exhibition**			
11:30 - 13:00	**Session V: Speciation in nutrition, environment and bioinorganic chemistry**			
13:00 - 14:00	**Lunch**			
14:00 - 16:10	**Session V continues: Speciation in nutrition, environment and bioinorganic chemistry**			
	Short Courses Session III			
16:15 - 18:00	**Short course C1**	**Short course C2**	**Short course C3**	**Short course C4**
18:00 - 18:15	**Coffee break, poster viewing and exhibition**			
	Short Courses Session IV			
18:15 - 20:00	**Short course D1**	**Short course D2**	**Short course D3**	**Short course D4**
From 19:00	**Dinner**			

Wednesday 17 June 2026

08:00 - 10:30	**Session VI: Laser ablation applications in spectrochemistry - microplastic and particulate analysis**
10:30 - 11:00	**Coffee break, poster viewing and exhibition**
11:00 - 12:30	**Session VII: Advances in nuclear and isotopic measurements**
12:30 - 13:30	**Lunch**
13:30 - 16:00	**Session VIII: Real time, in situ and other measurements**
16:30 - 23:00	**Departure for excursion to the Briksdalen Glacier with a conference outdoor dinner**

Thursday 18 June 2026

08:30 - 09:45	**Poster viewing, exhibition and discussions with morning coffee and tea**
09:45 - 11:30	**Poster viewing, exhibition and discussions with morning coffee and tea**
11:30	**Short course: Analytical nano-material characterisation**
12:00	**Closing remarks and farewell**
	Lunch

11 Daily Programme

Sunday 14 June 2026

08:45-09:15 **Welcome/Opening remarks**
Yngvar Thomassen

Session I: Frontiers in atomic and molecular spectrochemistry

Chair: R. Kenneth Marcus

09:15-09:45 **O-1** **(Quasi) Simultaneous atomic and molecular spectrometry – Past, present, and possible future**
Gary M. Hieftje
Department of Chemistry, Indiana University, Bloomington, USA

09:45-10:15 **O-2** **Measurement science & governance: Shaping national and international policy**
Vahid Majidi,
Independent, Aiken, South-Carolina, USA

10:15-10:45 **O-3** **Renaissance of nitrogen as an alternative gas for inductively coupled plasma mass spectrometry**
Monique Kuonen, Dylan Käser, Joachim Koch, Bodo Hattendorf and Detlef Günther
ETH Zurich, Department of Chemistry and Applied Biosciences, Zurich, Switzerland

10:45-11:15 **O-4** **Novel types of applications are driving a never-ending demand for improved ICP-MS capabilities**
Frank Vanhaecke, Rinus Dejonghe, Mina Nikolic, Thibaut Van Acker and Ana Lores-Padin
Atomic & Mass Spectrometry – A&MS research unit, Department of Chemistry, Ghent University, Belgium

11:15-11:45 **Coffee, exhibition and poster viewing**

11:45-12:05 **O-5** **Collision-induced isotope fractionation in ICP-MS/MS under He, Ne, and Ar condition**
Kengo Ito[1,2], Chihaya Kinoshita[1], Toshiyuki Fujii[2] and Takafumi Hirata[1]
[1] Geochemical Research Center, Graduate School of Science, The University of Tokyo, Japan
[2]Division of Sustainable Energy and Environmental Engineering, Graduate School of Engineering, the University of Osaka, Japan

12.05-12:25 **O-6** **Isotopic fractionation of zirconium through ion reactions with NH_3 found in inductively coupled plasma–tandem mass spectrometry**
Hiroaki Takahashi[1], Kota Yamamoto[1], Chihaya Kinoshita[2], Kengo Ito[2] and Takafumi Hirata[2]
[1] Regulatory Standard and Research Department, Secretariat of Nuclear Regulation Authority, Tokyo, Japan
[2] Geochemical Research Center, Graduate School of Science, The University of Tokyo, Japan

12:25-12:45 **O-7** **Detection of volatile organic compounds through soft ionisation using ICP-tandem mass spectrometry (ICP-MS/MS)**

Takafumi Hirata[1], Chihaya Kinoshita[1,2] and Ritsu Morisaki[1],
[1] *Geochemical Research Center, Graduate School of Science, The University of Tokyo, Japan*
[2] *Present affiliation: ST Japan IncChuo-ku, Tokyo, Japan.*

13:00 **Lunch**

14:00 **Excursion to Geiranger and Loen Lake**

Other activities: Loen Skylift and the Skåla Challenge

From 19:00 **Dinner**

Monday June 15 2026

Session II: Progress in instrumentation and application of spectrochemistry

Chair: Jens Sloth

08:00-08:30 **O-8** **Multi-pressure approach and X-ray desorption of solid reagent precursors for sustainable chemical ionization mass spectrometry**
Aleksei Scherbinin
Karsa OY and University of Helsinki, Helsinki, Finland

08:30-08:50 **O-9** **Optimising ICP-MS analysis: Enhancing helium collision and reaction cell modes**
Naoki Sugiyama[1], Michiko Yamanaka[1], Erina Shimizu[1] and Raimund Wahlen[2]
[1] Agilent Technologies Japan, Ltd., 9-1 Takakura-machi, Hachioji-shi, Tokyo 192-8510, Japan
[2] Agilent Technologies UK Ltd, 5500 Lakeside, Cheadle Royal Business Park, Stockport, SK8 3GR, UK

08:50-09:10 **O-10** **The Avio 3000: The first third-generation ICP-OES platform built around fundamental redesign**
Minyu Zuo[1] and Daniel Fliegel[2]
[1] PerkinElmer Nordics
[2] PerkinElmer Norway AS

09:10-09:30 **O-11** **Fast analysis of environmental samples by ICP-QQQ with discrete sampling**
Satoshi Kondo[1], Michiko Yamanaka[1], Glenn Woods[2] and Raimund Wahlen[2]
[1] Agilent Technologies Japan, Ltd., 9-1 Takakura-machi, Hachioji-shi, Tokyo 192-8510, Japan
[2] Agilent Technologies UK Ltd, 5500 Lakeside, Cheadle Royal Business Park, Stockport, SK8 3GR, UK

09:30-09:50 **O-12** **Innovative multielement analysis strategies for occupational airborne metals: ICP-MS and complementary techniques**
Tobias Schwank, J. Heck, M. Krämer and C. Wippich
Institute for Occupational Safety and Health of the German Social Accident Insurances – IFA, Sankt Augustin, Germany

09:50 – 10:10 **O-13** **Extending the analytical reach of ICP-OES: UV boost mode on the Avio 3000 for the determination of crucial challenging low-UV elements**
Minyu Zuo[1] and Daniel Fliegel[2]
[1] PerkinElmer Nordics
[2] PerkinElmer Norway AS

10:10-10:40 **Coffee break, exhibition and poster viewing**

Session III: Ionisation, laser ablation and elemental/molecular imaging

Chair: Ewa Bulska

10:40-11:10 **O-14** **Microplasma ionization coupled to enhanced orbitrap mass spectrometers: Moving towards elemental and isotopic analysis *without* chemical separation**
R. Kenneth Marcus
Clemson University, Clemson, USA

11:10-11:40 **O-15** **Elemental imaging by mass spectrometry at the micro and nanoscale - Challenges and prospects**
Dirk Schaumlöffel
CNRS/Université de Pau et des Pays de l'Adour, Pau, France

11:40-12:10 **O-16** **Understanding the role of ion charge and size in their susceptibility to acoustic ion manipulation (AIM)**
Jacob T. Shelley,[1] Julia L. Danischewski,[1] Joshua S. Wiley,[2] Yi You,2 Josefin Hufgard,[2] and Jens Riedel[2]
[1] Department of Chemistry and Chemical Biology, Rensselaer Polytechnic Institute, Troy, NY, USA
[2] Department of Instrumental Analytics, Federal Institute for Materials Research and Testing (BAM), Berlin, Germany

12:10-12:40 **O-17** **Laser ablation with simultaneous elemental and molecular mass spectrometry imaging: From plant samples to tattoos**
Uwe Karst, Johannes Schmeinck, Lea Tobergte, Till Schröder, Lena Hiddeßen, Lena Schlautmann, Mark Wesner, Hannah Freyer and Katharina Kronenberg
Institute of Inorganic and Analytical Chemistry, University of Münster, Germany

12:40-13:00 **O-18** **Multimodal bioimaging using mass spectrometric and spectroscopic techniques on a single tissue thin section**
Lena Hiddeßen[1], Lea Würfel[2], Rickmer Braren[2,3], Irina Heid[2] and Uwe Karst[1]
[1] Institute of Inorganic and Analytical Chemistry, University of Münster, Germany
[2] Institute of Diagnostic and Interventional Radiology, TUM University Hospital Rechts der Isar, Technical University of Munich, Germany
[3] Department of Diagnostic and Interventional Radiology and Nuclear Medicine, University Medical Center Hamburg-Eppendorf, Hamburg, Germany

13:00-14:00 **Lunch**

Session III continues: Ionisation, laser ablation and elemental/molecular imaging

Chair: Dirk Schaumlöffel

14:00-14:30 **O-19** **Mapping strategies and calibration approaches for laser ablation ICP-MS imaging**
Martin Šala
National Institute of Chemistry, Ljubljana, Slovenia

14:30-14:50 **O-20** **Hyphenation of laser ablation with ICP-MS and APCI-MS for simultaneous elemental and molecular imaging of flower buds from the invasive narrow leaved ragwort**
Till Schröder, J. Schmeinck and U. Karst
University of Münster, Institute of Inorganic and Analytical Chemistry, Germany

14:50-15:10 **Presentation of MiMac: From materials to minerals – orthogonal expertise across the critical supply chain**
Debora Foppiano
SINTEF Industry, Trondheim, Norway

Short Courses Session I

15:20-17:05	**A1-A5**	**A1**	**A2**	**A3**	**A4**	**A5**
		Jörg Bettmer:	Lukas Brunnbauer:	Rainer Cramer:	Benjamin Manard:	Frank Vanhecke:
		Tracing nanomaterials in biological systems: A brief overview on sample preparation and characterisation techniques	**An introduction to machine learning for sample classification based on elemental fingerprinting**	**Development and applications of ion sources in biological MS**	**Nuclear material characterization: Tools, techniques, and emerging capabilities**	**An introduction to isotopic analysis**

17:05-17:30 **Coffee break, exhibition and poster viewing**

Short Courses Session II

17:30-19:15	**B1-B5**	**B1**	**B2**	**B3**	**B4**	**B5**
		Detlef Günther:	Karl A. Jensen:	Heidi-Goenaga-Infante:	Dirk Schaumlöffel:	Nicole Strittmatter and Zoltan Takats:
		Workshop on laser ablation-ICP-mass spectrometry	**Practical approaches to the use of reaction gases in triple quadrupole ICP-MS**	**Metrological and standardisation advances for particle concentration: From inorganic nanomaterials to bio-nanoparticles to microplastics**	**Secondary ion mass spectrometry for elemental and isotopic imaging**	**Ambient ionization mass spectrometry**

From 19:00 **Dinner**

21:00 **BYOB gathering with exhibition, poster viewing and discussions (*remember to bring your drink of choice*)**

Tuesday 16 June 2026

Session IV: Molecular and biological mass spectrometry imaging

Chair: Uwe Karst

08:00-08:30 **O-21** **Liquid atmospheric pressure MALDI – a multifunctional ionisation technique for biological mass spectrometry**
Rainer Cramer
Department of Chemistry, University of Reading, UK

08:30-09:00 **O-22** **Rapid evaporative ionization mass spectrometry: From mechanistic insights to subcellular resolution**
Zoltan Takats
Imperial College, London, UK and University of Regensburg, Germany

09:00-09:30 **O-23** **Desorption electrospray ionization mass spectrometry: Recent developments for highly sensitive and detailed imaging of biological samples**
Christian Janfelt
Department of Pharmacy, University of Copenhagen

09:30-10:00 **O-24** **Molecules in space and time**
Luca Varga, Daniel Horvath, Eva Amara Ung and Laszlo Mark
University of Pecs, Hungary

10:00-10:30 **Coffee break, exhibition and poster viewing**

10:30-11:00 **O-25** **Direct infusion tools for spatial and cellular metabolomics**
Ingela Lanekoff
University of Uppsala, Sweden

11:00-11:20 **O-26** **Mass spectrometry-based omics sciences for precision medicine and risk assessment of modern therapeutics**
Ewa Bulska
University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Warsaw, Poland

Session V: Speciation in nutrition, environment and bioorganic chemistry

Chair: Heidi Goenaga-Infante

11:30-12:00 **O-27** **The role of ICP-MS and other MS-techniques in the characterization of biogenic selenium nanoparticles in mushrooms**
Jörg Bettmer A. Suárez Priede, M. Corte Rodríguez and P. Díez García
University of Oviedo, Dept. of Physical and Analytical Chemistry, Oviedo, Spain
Health Research Institute of the Principality of Asturias (ISPA), Oviedo, Spain

12:00-12:20 **O-28** **Analysis of gadolinium-based contrast agent uptake in brain cell cultures using IC-ICP-MS**
Victoria Kazimierczyk[1], L. Pusch[2], L. M. Müller[2], V. Michaelis[2], J. Bornhorst[2] and U. Karst[1]
[1] University of Münster, Institute of Inorganic and Analytical Chemistry, Germany
[2] University of Wuppertal, Faculty of Mathematics and Natural Sciences, Wuppertal, Germany

12:20-12:40 **O-29** **From molecules to elements: Electrospray ionization coupled to high resolution mass spectrometric for trace element speciation**
Damiano Monticelli[1], Alejandro Ruiz López[1,2], Gianluca Roncoroni[1]
[1] Dipartimento di Scienza e Alta Tecnologia, University of Insubria, Como, Italy
[2] Scuola Universitaria Superiore Pavia IUSS, Pavia, Italy

12:40-13:00 **O-30** **Mercury and selenium isotopic analysis for unraveling Hg detoxification mechanisms in marine biota**
Mathias Vandermeiren[1], L. Abou-Zeid[1], L. Suarez-Criado[1], Martin Wiech[2] and F. Vanhaecke[1]
[1] *Ghent University, Department of Chemistry, Ghent, Belgium*
[2] *Institute of Marine Research, Bergen, Norway*

13:00-14:00 **Lunch**

Session V continuous: Speciation in nutrition, environment and bioorganic chemistry

Chair: Heidi Goenaga-Infante

14:00-14:30 **O-31** **Fate of gadolinium-based contrast agents in the body and environment: Insights from speciation studies**
Ryszard Lobinski,[1] Izabela Strzemińska,[2] Cécile Factor,[2] Celia Trujillo,[1,3] Francisco Laborda[3] and Javier Jimenez-Lamana[1]
[1] *CNRS, Institute of Analytical and Physical Chemistry for the Environment and Materials (IPREM - UMR 5254), Pau, France*
[2] *Guerbet Research and Innovation Department, Aulnay-sous-Bois; France*
[3] *Universidad de Zaragoza, Department of Chemistry, Zaragoza, Spain*

14:30-15:00 **O-32** **The dark side of ICP-MS: Negative ions for fluorine, PFAS, and beyond**
Jörg Feldmann, Viktoria Müller, Andrea Raab and Raquel Gonzalez de Vega
TESLA-Analytical Chemistry, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

15:00-15:20 **O-33** **Unravelling the mechanism of glyphosate formation from aminopolyphosphonates by hyphenation of ion chromatography to ICP-MS and ESI-MS**
Mathis Athmer[1], Anna M. Röhnelt[2], Stefan B. Haderlein[2] and Uwe Karst[1]
[1] *Institute of Inorganic and Analytical Chemistry, University of Münster, Germany*
[2] *Geo-and Environmental Research Center, Department of Geosciences, University of Tübingen, Tübingen, Germany*

15:20-15:50 **O-34** **Examples of trace element speciation analysis in foodstuffs – from research to regulation**
Jens Sloth
Technical University of Denmark, Lyngby, Denmark

15:50-16:10 **O-35** **New insights into the speciation of small organically - bound chromium species at low µg kg^{-1} concentrations in collected aerosols from e-cigarettes using HPLC-ICP-MS**
Serhat Doker, John Entwisle, Kyle Saunders, Luise Luckau and Heidi Goenaga-Infante
National Measurement Laboratory, LGC, Guildford, UK

Short Courses Session III

16:15-18:00	**C1 - C4**	**C1** Jorge Pisonero: **Introduction to GD-MS for direct analysis of innovative materials**	**C2** Jörg Feldmann and Victoria Müller: **Fluorine and PFAS analysis – Linking molecular and elemental detection**	**C3** Uwe Karst: **Laser ablation and molecular mass spectrometry: Fundamentals and applications**	**C4** Laslo Márk: **Matrix-assisted laser desorption-ionization (MALDI)-MS: A powerful mass spectrometry imaging technique**
18:00-18:15		**Coffee break, exhibition and poster viewing**			

Short Courses Session IV

18:15-20:00	**D1 - D4**	**D1** Ryszard Lobinski: **Plasma source mass spectrometry for trace element speciation analysis: from principles to practice**	**D2** R. Kenneth Marcus: **Orbitrap mass analyzers for elemental and isotopic analysis**	**D3** Martin Šala: **LA-ICP-MS mapping: from fundamentals to high resolution calibrated elemental maps**	**D4** Jacob T. Schelley: **Direct molecular mass spectrometry with atmospheric pressure plasmas**
From 19:00		**Dinner**			

Wednesday 17 June 2026

Session VI: Laser ablation applications in spectrochemistry – microplastic and particulate analysis

Chair: Jacob T. Shelley

08:00-08:30 **O-36** **Laser ablation based spectroscopy: From multi-elemental tissue mapping to unveiling segregation phenomena in metallurgy**

Jorge Pisonero[1], C. Soto[1], A. Méndez[2], A. Calon[3], J. Linares[3], I. García[4], H. Kopřivová[5], J. Orejas[1] and N. Bordel[1]

[1]Department of Physics, Faculty of Science, University of Oviedo, Spain
[2]Servicios Cientifico Técnicos, University of Oviedo, Spain
[3]Hospital del Mar Medical Research Institute (IMIM), Barcelona, Spain
[4]Know-How Innovative Solutions and Manufacturing, Gijón, Spain.
[5]Central European Institute of Technology (CEITEC), Brno, Czech Republic

08:30-09:00 **O-37** **Detection and characterization of microplastics by LA-ICP-MS and LIBS**
Lukas Brunnbauer and Andreas Limbeck
TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria

09:00-09:30 **O-38** **A multi-method platform for the characterization of microplastics: From pristine materials to complex samples**
Heidi Goenaga-Infante
National Measurements Laboratory, LGC, UK

09:30-09:50 **O-39** **Development of a multimethod platform based on laser direct infra-red (LD-IR) imaging spectroscopy for the reliable identification and characterisation of microplastics**
Aneta Sikora, David Ojeda, Dorota Bartczak and Heidi Goenaga-Infante
National Measurement Laboratory hosted at LGC, Guilford, UK

09:50-10:10 **O-40** **Establishing a random forest classifier based on LIBS for process control of galvannealed steel strip**
Jakob Willner[1], David K. Gibbs[1], Lukas Brunnbauer[1], Fabian Friedl[2] and Andreas Limbeck[1]
[1] *TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria*
[2] *Voestalpine Stahl GmbH, Linz, Austria*

10:10-10:30 **O-41** **How can various ICP-MS techniques provide complementary information on nanogold alterations?**
Magdalena Matczuk, K. Nowak and M. Mierzwa
Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland

10:30-11:00 **Coffee break, exhibition and poster viewing**

Session VII: Advances in nuclear and isotopic measurements

Chair: Vahid Majidi

11:00-11:30 **O-42** **Single-particle ICP-MS: New frontiers in uranium particle analysis**
Benjamin T. Manard
Oak Ridge National Laboratory, Oak Ridge, USA

11:30-11:50 **O-43** **Calibration approaches for radionuclide measurements by ICP-MS/MS**
Valeriia Morozova, Karl Andreas Jensen and Deborah H. Oughton
Norwegian Nuclear Research Centre, NMBU, Ås, Norway

11:50-12:10 **O-44** **Miniaturized solid-phase extraction – inductively coupled plasma mass spectrometry (mini-SPE-ICP-MS) coupling for U/Pu determination**
Antonia Toska,[1] Hélène Isnard[1] and Carole Bresson[1]
[1] *Université Paris-Saclay, CEA, Service de Physico-Chimie, Gif-sur-Yvette, France*

12:10-12:30 **O-45** **Isotopic and elemental composition analysis of historical artifacts to enhance the interpretation of past research findings**
Jakub Karasiński[1], Klaudia Tetfejer[1], Ewa Bulska[1], Piotr Radziński[2], Kamil Nowak[3] and Barbara Wagner[1]
[1] *University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Warsaw, Poland*
[2] *University of Warsaw, Institute of Informatics, Warsaw, Poland*
[3] *Austrian Archaeological Institute, Austrian Academy of Sciences, Vienna, Austria*

12:30-13:30 **Lunch**

Session VIII: Real-time, in situ and other measurements

Chair: Jörg Feldmann

13:30-14:00 **O-46** **Proton-transfer-reaction mass spectrometry (PTR-MS): Fundamentals and applications in real-time VOC monitoring**

Nikita Sobolev, Felix Benjamin Blixt Hasle, Keerthana Balashankar, Tomas Mikoviny and Armin Wisthaler
Department of Chemistry, University of Oslo, Norway

14:20-14:40 **O-47** **Shredding of lithium ion batteries: Investigating material degradation and safety**

J. Buchmann[1], C. Peschel[1], M. Winter[1,2], S. Wiemers-Meyer[1] and Sasha Nowak[1]
[1] University of Münster, MEET Battery Research Center, Münster, Germany
[1] Helmholtz-Institute Münster, IEK-12, Forschungszentrum Jülich GmbH, Münster, Germany

14:40-15:00 **O-48** **Correlative imaging workflow combining LA-ICP-MS and IR spectroscopy for gadolinium mapping in neural tissue**

Hannes Gödde[1], Hennes Rave[2], Astrid Jeibmann[3,4], Lars Linsen[2] and Uwe Karst[1]
[1] Institute of Inorganic and Analytical Chemistry, University of Münster, Germany
[2] Institute of Informatics, University of Münster, Germany
[3] Clinic of Radiology, University of Münster, Germany
[4] Diagnostic Imaging Research Unit (DIRU), Clinic for Diagnostic Imaging, Vetsuisse Faculty, University of Zurich, , Switzerland

15:00-15:20 **O-49** **Advancing fragmentology by multi-technique spectrometric analysis**

Barbara Wagner[1], Jakub Karasiński[1], Ludwik Halicz[1], Piotr Targowski[2], Dorota Jutrzenka-Supryn[3] and Monika Opalińska[4]
[1] Faculty of Chemistry, University of Warsaw, Poland
[2] Institute of Physics, Nicolaus Copernicus University in Toruń, Poland
[3] Faculty of Fine Arts, Nicolaus Copernicus University in Toruń, Poland
[4] Faculty of Modern Languages, University of Warsaw, Poland

15:20-15:40 **O-50** **Hidden fluorine in gasoline: Multi-technique detection of fluorinated species coming from alkylation processes**

Viktoria Müller [1, 2], Markus Rotzinger [2], Zofia Kowaleswka [3], Raquel Gonzalez de Vega [2], Klaus Zangger [2] and Jörg Feldmann [2]
[1] The James Hutton Institute, Craigiebuckler, Aberdeen, United Kingdom
[2] University of Graz, Austria
[3] Faculty of Civil Engineering, Mechanics and Petrochemistry, Warsaw University of Technology, Płock, Poland

15:40-16:00 **O-51** **Assessment of metal contamination in cannabis inflorescences and the impact of consumer preparation tools**

Jan Piecuch[1,2], Ewelina Pollak-Kowa[1,2], Marcin Wieczorek[1] and Anna Telk[1]
[1] Faculty of Chemistry, Department of Analytical Chemistry, Jagiellonian University, Kraków, Poland
[2] Doctoral School of Exact and Natural Sciences, Jagiellonian University, Kraków, Poland

16:30 **Departure for the excursion to the Briksdal Glacier with a conference outdoor dinner**

Thursday 18 June 2026

08:30-09:45 **Poster viewing, discussions and exhibition with morning coffee and tea**

09:45-11:30

Short course:

(E-1)

Analytical nano-material characterization

Vahid Majidi

National Security, Aitken, USA

11:30 **Closing remarks and farewell**

12:00 **Lunch**

Poster Presentations
Sunday 14 June - Thursday June 18 2026

P-1 **Development of a certified water reference material to support laboratory measurement traceability**

Anna Ruszczyńska, Jakub Karasiński, Andrzej Gawor and Marcin Wojciechowski
University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Warsaw, Poland

P-2 **How plasma-based analysis techniques enhance battery research.**

Alexandros Tsoufios[1], D. Kessen[1], J. M. Dressler[1], J. Busch[1], M. Winter[1,2], S. Wiemers-Meyer[1] and S. Nowak[1]
[1] *MEET Battery Research Center, University of Münster, Münster, Germany*
[2] *Helmholtz-Institute Münster, IMD-4, Forschungszentrum Jülich GmbH, Münster, Germany*

P-3 **Fluorine depth profiling of lithium ion battery electrodes *via* glow discharge-sector field-mass spectrometry**

S.L. Dorn[1], B. Sienknecht[1], J. Kauling[1], M. Börner[1], Winter, M.[1,2], S. Wiemers-Meyer[1] and S. Nowak[1]
[1] *University of Münster, MEET Battery Research Center, Münster, Germany*
[2] *Helmholtz-Institute Münster, IMD-4, Forschungszentrum Jülich GmbH, Münster, Germany*

P-4 **Application of ICP-MS for multi-element analysis of iodine and trace elements in brown seaweed: A seasonal study of Fucus vesiculosus**

Dong Han[1], Ditte B. Hermund[1], Julie S. Vikkelsø[1], Gonçalo S. Marinho[1,2], Jens J. Sloth[1] and Susan L. Holdt[1]
[1] *Technical University of Denmark, National Food Institute, Kgs. Lyngby, Denmark*
[2] *CIIMAR/CIMAR LA, Centro Interdisciplinar de Investigação Marinha e Ambiental, Universidade*
do Porto, Terminal de Cruzeiros do Porto de Leixões, Matosinhos, Portugal

P-5 **Assessing sodium plating and transition metal deposition on hard carbon anodes in commercial sodium ion batteries by means of plasma-based techniques**

Jannis Busch [1], Alexandros Tsoufios [1], Martin Winter [1,2], Simon Wiemers-Meyer [1] and Sascha Nowak [2]
[1] *University of Münster, MEET Battery Research Center, Münster, Germany*
[2] *Helmholtz-Institute Münster, IEK-12, Forschungszentrum Jülich GmbH, Münster, Germany*

P-6 **ICP-TOF-MS and HRAM-MS in the field of battery research, production and recycling – from single particle analysis to molecular imaging**

J. M. Dressler, S. Nowak, M. Winter and S. Wiemers-Meyer
University of Münster, MEET Battery Research Center, Münster, Germany

P-7 **Investigating the diversity in arsenic speciation in mushrooms**

Julia Truschner[1,2], Lorenz Steiner[1], Andrea Raab[3], Jan Borovicka[4,5], Walter Goessler[1] and Bassam Lajin[1,2]
[1] *Institute of Chemistry, Analytical Chemistry for the Health and Environment, University of Graz, Austria*
[2] *Institute of Chemistry, ChromICP, University of Graz, Austria*
[3] *Institute of Chemistry, TESLA, University of Graz, Austria*
[4] *Institute of Geology, the Czech Academy of Sciences, Prague, Czech Republic*
[5] *Nuclear Physics Institute, the Czech Academy of Sciences, Husinec-Řež, Czech Republic*

P-8 **Is arsenic essential?**
Helen Lord,[1] Fernando Mendoza[2], Joerg Feldmann[1] and Viktoria Mueller[1]
[1] *Karl-Franzens University of Graz, Austria*
[2] *Technical University of Graz, Austria*

P-9 **Temperature-programmed desorption / pyrolysis coupled to direct analysis in real time Fourier Transform ultrahigh resolution orbitrap mass spectrometry for the analysis of natural organic matter**
Ilwan Meignant[1], Marios Drosos[2] and Maxime C. Bridoux[1]
[1] *CEA, DAM, DIF, F-91297 Arpajon, France*
[2] *Department of Agricultural, Forest, Food and Environmental Sciences, University of Basilicata, Potenza, Italy*

P-10 **Elemental interference uncovered: How alkali and alkaline earth metals influence $[BaF]^+$ and $[SrF]^+$ Methods for fluorine analysis using ICPMS/MS**
Franziska Peer[1], Andrea Raab[1], Raquel Gonzalez de Vega[1] and Jörg Feldmann[1]
[1] *University of Graz, Institute of Chemistry, TESLA- Analytical Chemistry, Graz, Austria*

P-11 **Determination of major and trace elements in plant-based foods by ICP-MS**
Liyan Xing[1], Aaron Hineman[1] and Daniel Fliegel[2]
[1] *PerkinElmer U.S. LLC*
[2] *PerkinElmer Norway AS*

P-12 **Elemental analysis of mining and soil samples by ICP-MS following aqua regia digestion**
Aaron Hineman[1] Minyu Zuo[2] and Daniel Fliegel[3]
[1]*PerkinElmer U.S. LLC*
[2]*PerkinElmer Nordics*
[3]*PerkinElmer Norway AS*

P-13 **Direct determination of trace impurities in high-purity molybdenum using the NexION 1100 ICP-MS**
Xiaoling Ma[1] Minyu Zuo[2] and Daniel Fliegel[3]
[1]*PerkinElmer China*
[2]*PerkinElmer Nordics*
[3]*PerkinElmer Norway AS*

P-14 **Ultra-trace elemental analysis of ultrapure water for semiconductor applications using the NexION 5000 multi-quadrupole ICP-MS**
Liyan Xing[1] Minyu Zuo[2] and Daniel Fliegel[3]
[1]*PerkinElmer China*
[2]*PerkinElmer Nordics*
[3]*PerkinElmer Norway AS*

P-15 **Determining hexavalent chromium species in air samples from occupational exposure using IC-ICP-MS**
Johanne Ø. Halvorsen**,** Nils Petter Skaugset, Mina Langfjord, Pål Graff and Torunn K. Ervik
STAMI, National Institute of Occupational Health, Oslo, Norway

P-16 **A statistical approach to homogeneity assessment of a multifunctional plant-based CRM for metal analysis**

Andrzej Gawor[1], Jakub Karasiński[1], Anna Ruszczyńska[1], Marcin Wojciechowski[1], A. Tupys[1], Aldona Kubala-Kukuś[2], Dariusz Banaś[2], J. Dobrzyńska[3], J. Reszko-Zygmunt[3], R. Dobrowolski[3] and Ewa Bulska[1]*

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[2] Jan Kochanowski University of Kielce, Faculty of Exact and Natural Sciences, Institute of Physics, Kielce, Poland

[3] Maria Curie-Skłodowska University, Faculty of Chemistry, Lublin, Poland

P-17 **Comprehensive mapping of the psoriatic skin proteome using mass spectrometry**

Andrzej Gawor[1], Anna Ruszczyńska[1], Olha Dushna[1], Karol Pniewski[2], Witold Owczarek[2] and Ewa Bulska[1]

[1] University of Warsaw, Faculty of Chemistry, Biological and Chemical Research Centre, Warsaw, Poland

[2] Institute of Medicine – National Research Institute, Department of Dermatology, Warsaw, Poland

P-18 **Single-cell ICP-MS for quantifying cisplatin uptake in veterinary-relevant cell models: Bridging application and instrumentation**

Balázs Berlinger[1], Gábor Andócs[1], Minyu Zou[2] and Csaba Kővágó[1]

[1]University of Veterinary Medicine, Budapest, Hungary

[2]PerkinElmer Nordics, Hägersten, Sweden

P-19 **Calibration of single-particle ICP-MS and its application on antibacterial products**

Wan-waan Lee[1] and Jingbo Chao[2]

[1] Government Laboratory of the Hong Kong Special Administration Region, Hong Kong, China

[2] Division of Chemical Metrology and Analytical Science, National Institute of Metrology, China

P-20 **Three-dimensional and immuno-mass spectrometry imaging of HfO_2 nanoparticles in breast cancer tissue by LA-ICP-TOFMS**

Lingna Zheng[1], Meng Wang[1], Weiyue Feng[1], Frank Vanhaecke[2]

[1] CAS Key Laboratory for Biomedical Effects of Nanomaterials and Nanosafety, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China

[2] Atomic & Mass Spectrometry - A&MS research group, Department of Chemistry, Ghent University, Ghent, Belgium

P-21 **Plasma-based CE-ICP-MS/MS study of formation and physiological alterations in cisplatin–gold nanoparticle delivery systems**

K. Nowak, D. Dąbrowski and M. Matczuk

Chair of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland

P-22 **Characterization of gold nanoparticle–cisplatin DDSs using two different CE–ICP-MS interfaces**

Damian Dąbrowski, Kinga Nowak and Magdalena Matczu

Chair of Analytical Chemistry, Faculty of Chemistry, Warsaw University of Technology, Warsaw, Poland

P-23 **Evaluating the bioaccessibility of trace metals in a plant based alternative protein source, canola meal, using online leaching method coupled to inductively coupled plasma mass spectrometry**

Yangyang Wang, Qiqi Zhang and Diane Beauchemin
Queen's University, Department of Chemistry, Kingston, Canada

P-24 **Agilent 9500 ICP-QQQ with m-lens for ultra-trace analysis of high-purity reagents**

Rentaro Yamashita[1], Raimund Wahlen[2] and Sonia North[2]
[1] Agilent Technologies International Japan, Tokyo, Japan 192-0033
[2] Agilent Technologies LDA, UK, Stocport, Cheshire, SK8 3GR, UK

P-25 **Analysis of high purity titanium using an Agilent 9500 ICP-QQQ**

Rentaro Yamashita[1], Raimund Wahlen[2] and Sonia North[2]
[1] Agilent Technologies International Japan, Ltd., 9-1 Takakura-machi, Hachioji-shi, Tokyo, Japan 192-0033
[2] Agilent Technologies LDA, UK, Stocport, Cheshire, SK8 3GR, UK

P-26 **Automation in trace metals analysis of engine coolants**

Luke Gormley[1], Sima Singha[1], Raimund Wahlen[2] and Sonia North[2]
[1] Agilent Technologies, Illinois, USA
[2] Agilent Technologies LDA, UK, Stocport, Cheshire, SK8 3GR, UK

P-27 **Enhancing lithium-ion battery production - Automated and sustainable elemental analysis using an ICP-OES**

Sima Singha, Ruby Bradford, Raimund Wahlen[2] and Sonia North[2]
[1] Agilent Technologies, Illinois, USA
[2] Agilent Technologies LDA, UK, Stocport, Cheshire, SK8 3GR, UK

P-28 **Microdroplets in quantitative LA-ICP-QMS: Application in depth resolved ion doping determination of semiconductors**

Jakob Willner[1], Maximilian Podsednik[2] and Andreas Limbeck[1]
[1] TU Wien, Institute of Chemical Technologies and Analytics, Vienna, Austria
[2] KAI Kompetenzzentrum für Automobil- und Industrieelektronik GmbH, ienna, Austria

P-29 **Investigation of *in vivo* Hg detoxification mechanisms by Se through elemental and isotopic analysis**

M. Vandermeiren[1], L. Abou-Zeid[1], L. Suarez-Criado[1], A. R. López[2,3], Martin Wiech[4] and F. Vanhaecke[1]
[1] Ghent University, Department of Chemistry, Atomic & Mass Spectrometry – A&MS research group, Ghent, Belgium
[2] University School for Advances Studies IUSS Pavia, Pavia, Italy
[3] Department of Science and High Technology., University of Insubria, Como, Italy
[4] Institute of Marine Research, Bergen, Norway

12 Oral Abstracts

(O-1)

(Quasi) Simultaneous atomic and molecular spectrometry – Past, present, and possible future

Gary M. Hieftje

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The more perceptive among those who read this abstract recognize already that a change in title of the former "Nordic Conference on Plasma Spectrochemistry" has occurred. The new name, "Nordic Conference on Plasma Spectrochemistry and Ionization Principles in Mass Spectrometry: From Elements to Molecules" is in keeping with an evolution that has gradually taken hold in the field of plasma-based analysis – in particular, from purely elemental analysis, to speciation analysis and, most recently, to metallomics and a full evaluation of BOTH the elemental and molecular composition of a sample. Most of these changes are reflected in lectures given at one or more of the earlier biennial versions of the conference. Naturally, this evolution has involved not only a gradual change in focus or application but also the introduction of new instrumentation and adaptation of existing systems. Some of these newer devices and means of utilization lie in the ionization source while others are found in the spectrometer. In this lecture, portions of this evolution in instrumentation will be traced, and compared with the current state of the art. This backdrop will then be used to suggest possible future devices and capabilities. As the title of this lecture suggests, the focus will be on simultaneous measurement of atoms, molecules, and molecular fragments, to permit elemental, molecular, and structural determination even for transient samples such as those produced by chromatography, laser or ion ablation, and thermal volatilization. In earlier systems, of course, measurements were sequential or parallel and only later were arrangements for simultaneous or extremely rapid (quasi-simultaneous) determination available.

(O-2)

Measurement science & governance: Shaping national and international policy

Vahid Majidi

Independant, Aiken, South-Carolina, USA

Over the past five decades, measurement science, particularly in the domain of analytical instrumentation, has undergone transformative development, fundamentally advancing both the qualitative and quantitative dimensions of scientific inquiry. These technological achievements, while often regarded primarily as technical milestones, have exerted a profound but underappreciated influence on the formulation of national policies and the dynamics of political decision-making.

This presentation examines the critical interface between measurement science and public policy, highlighting how objective, instrument-derived data serve not only as the evidentiary foundation for policy formulation but also as catalysts for political debate and unintended societal repercussions.

Focusing on environmental regulation and nuclear waste disposition, with illustrative case studies from the United States and Norway, this work illustrates the impact of analytical precision, reliability, and data timeliness on policy outcomes. Particular attention is directed toward the temporal dimension of data acquisition, underscoring how the immediacy and credibility of measurement results significantly influence regulatory responsiveness and the effectiveness of policy implementation.

(O-3)

Renaissance of nitrogen as an alternative gas for inductively coupled plasma mass spectrometry

Monique Kuonen, Dylan Käser, Joachim Koch, Bodo Hattendorf and Detlef Günther,

ETH Zurich, Department of Chemistry and Applied Biosciences, Vladimir Prelog Weg 1, 8093 Zurich, Switzerland

The introduction of a new nitrogen-ICP-OES system (MICAP) by the Hieftje group in 2017 [1] together with Radom AG (Milkwakee, USA) created a renaissance of the microwave-powered nitrogen plasma, which had been used already in the middle of the 70s in atomic spectroscopies [2]. Yet, at that time, the performance as ion source for mass spectrometry was not sufficiently competitive to the already than established Argon plasmas. Thus, in depth studies, which would have been required for a broader use of such a plasma source, remained scarce.

The compact ion source and the use of conventional Fassel-type torches of the MICAP may open a route for a transportable ICP-MS. In this sense, the plug-and-play approach allowing integration into common Argon-ICPMS infrastructure helped us to realize a prototype in combination with a TOFMS [3]. Due to the very complementary results achieved when compared to an Argon-based plasma mass spectrometer of the same type, a prototype quadrupole version was built. This instrument has been used for a thorough evaluation of a MICAP for routine analyses of liquids, solids, and nanomaterials [4-7]. Some of these findings and major advantages of the nitrogen plasma will be discussed.

Furthermore, the coupling of the MICAP with laser ablation sampling allows for sampling of aerosols generated in nitrogen or even air. By using only nitrogen, similar performance was achieved without the need for helium as carrier gas [8]. Various experiments using He/N_2 and N_2 only have been carried out to gain a better understanding of fundamental particle formation processes in nitrogen and air as a potential carrier gas. These results together with some revisited phenomena from He/Ar, He/N2 as well as some quantitative data will be presented.

[1] A. J. Schwartz, Y. Cheung, J. Jevtic, V. Pikelja, A. Menon, S. J. Ray and G. M. Hieftje, *J. Anal. At. Spectrom.*, 2016, **31**, 440–449
[2] C.I.M. Beenakker, *Spectrochim. Acta, Part B* 1976, **31**, 483− 486
[3] M. Schild, A. Gundlach-Graham, A. Menon, J. Jevtic, V. Pikelja, M. Tanner, B. Hattendorf and D. Günther, *Anal.*
[4] C. Neff, P. Becker, B. Hattendorf and D. Günther, *J. Anal. At. Spectrom.,* 2021, **36**, 1750-1757
[5] M. Kuonen, G. Niu, B. Hattendorf and D. Günther, *J. Anal. At. Spectrom.,* 2023, **38**, 758-765
[6] M. Kuonen, B. Hattendorf and D. Günther, *J. Anal. At. Spectrom*., 2024, **39**, 1388-1397
[7] M. Kuonen, B. Hattendorf and D. Günther, Talanta 2026, re-submitted
[8] D. Käser, J. Koch, B. Hattendorf, Th. v. Acker, D. Günther (in preparation)

(O-4)

Novel types of applications are driving a never-ending demand for improved ICP-MS capabilities

Frank Vanhaecke, Rinus Dejonghe, Mina Nikolic, Thibaut Van Acker and Ana Lores-Padin

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ICP-mass spectrometry shows sufficient sensitivity to quantitatively determine the amount (mass) of an essential mineral element at the single-cell level.[1,2] This can be accomplished either by introducing a dilute cell suspension using pneumatic nebulization or by using laser ablation for single-cell interrogation. These approaches enable the heterogeneity within a cell population to be characterized.

In this context, the use of an ICP-MS instrument equipped with a time-of-flight (ToF) analyzer is highly recommendable owing to the (quasi-)simultaneous monitoring offered by this type of instrumentation. The monitoring of a "marker element" – either an endogenous element with a sufficiently high content (e.g., Fe in RBCs[3]) or an exogenous element (e.g., introduced via an Ir-tagged DNA-intercalator[4]) – guarantees that each cell event is detected, thereby avoiding the result for endogenous elements present at lower content to be biased low. The (quasi-)simultaneous monitoring of the entire elemental mass spectrum also enables inter-element correlations to be studied at the level of individual cells and should allow access to isotope ratios.

However, as the continuous ion beam originating from the ICP ion source is only part-wise sampled for ToF-based mass analysis, ToF-ICP-MS lacks some detection capabilities when compared to quadrupole-based or sector-field ICP-MS. Overpulsing and isotope summation can improve the situation to some extent.[5] Still, ToF-ICP-MS instrumentation with improved limits of detection and quantification would be highly welcome.

In this presentation, recent single-cell ICP-MS analysis work carried out within the UGent-A&MS team will be discussed and the benefits of ToF-ICP-MS in this context demonstrated. Capabilities and limitations of such approaches will be illustrated at hand of real-life applications.

1. T. Liu, E. Bolea-Fernandez, O. De Wever and F. Vanhaecke, Analytica Chimica Acta, 1177, paper nr. 338797, 2021. DOI: 10.1016/j.aca.2021.338797.
2. R. Dejonghe, E. Bolea-Fernandez, A. Lores-Padin, T. Van Acker, A. Rua-Ibarz, O. De Wever and F. Vanhaecke, Microchemical Journal, 207, paper nr. 112013, 2024. DOI: 10.1016/j.microc.2024.112013.
3. R. Dejonghe, A. Lores-Padin, E. Bolea-Fernandez, T. Van Acker, O. De Wever and F. Vanhaecke, Spectrochimica Acta B, 236, paper nr. 107384, 2026. DOI: 10.1016/j.sab.2025.107384.
4. M. Nikolić, A. Lores-Padin, T. Van Acker, T. Smets, I. Goemaere, A. Ahmad, K. Braeckmans, E. Bolea-Fernandez and F. Vanhaecke, Talanta, 297, paper nr. 128696, 2025. DOI: 10.1016/j.talanta.2025.128696.
5. M. Nikolić, A. Lores-Padin, R. Dejonhe, Olivier De Wever and F. Vanhaecke, Talanta, submitted.

(O-5)

Collision-induced isotope fractionation in ICP-MS/MS under He, Ne, and Ar condition

Kengo Ito[1,2], Chihaya Kinoshita[1], Toshiyuki Fujii[2] and Takafumi Hirata[1]

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[2] Division of Sustainable Energy and Environmental Engineering, Graduate School of Engineering, the University of Osaka, Suita, Osaka 565-0871, Japan
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Isotope ratio measurements using inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) are generally interpreted based on mass-dependent fractionation (MDF), which is commonly corrected using power law or exponential law formulations [1]. However, gas-phase processes in the collision/reaction cell can introduce additional fractionation effects that are not fully understood, particularly after ion–molecule or collision-induced reactions. To address this issue, we investigated isotope fractionation behaviors of Mo, Hf, W, Sn, and Ru through the collisions with He, Ne, and Ar. The isotope ratios were evaluated relative to a reference isotope for each element, and their deviations from MDF behavior were examined.
In the collision with He, the measured isotope ratios exhibited systematic deviations from smooth MDF trends, including pronounced odd–even variations for several elements. These features were particularly evident for Mo and W, whereas Sn and Ru showed smaller but discernible deviations. In contrast, isotope fractionation patterns obtained under Ne and Ar conditions were significantly smoother and largely consistent with conventional MDF behavior. The magnitude of isotope fractionation was found to be element-dependent, following the order Mo ≈ W ≈ Hf > Sn ≳ Ru. In addition, variations in both the magnitude and sign of fractionation were observed depending on instrumental conditions, suggesting that multiple processes contribute to the observed isotope fractionation.
These results indicate that collision-induced processes in ICP-MS/MS can lead to non-MDF isotope fractionation, particularly under He conditions. Such behavior may reflect incomplete thermalization of ions and energy-dependent ion transmission within the collision cell. The observed element dependence further suggests that electronic structure plays a role in governing isotope fractionation during gas-phase collisions. In this presentation, we discuss the mechanisms of isotope fractionation during collision processes and their implications for high-precision isotope ratio measurements.

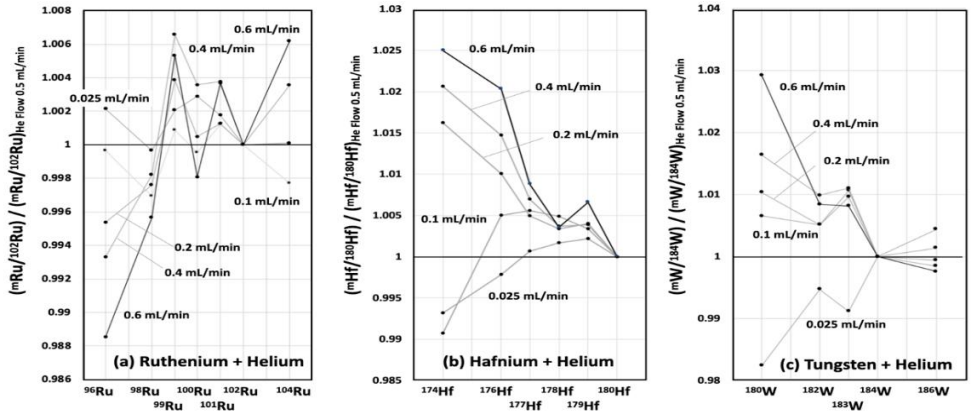

Figure 1 Isotope effect on Ru, Hf and W obtained through collisions with a different He inlet rate using ICP-MS/MS.

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(O-6)

Isotopic fractionation of zirconium through ion reactions with NH_3 found in inductively coupled plasma-tandem mass spectrometry

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The detection of trace amounts of the radioactive nuclide ^{93}Zr is a major issue for ensuring careful and reliable safety assessments in the complex decommissioning processes of nuclear facilities. Isotope dilution mass spectrometry (IDMS) has been widely employed to determine Zr isotopes because of its high repeatability and reliability. Minimizing various mass spectrometric interferences is crucial for improving data quality in Zr isotopic ratio measurements, particularly for determining ^{93}Zr, as notable measurement errors can be induced by isobaric interferences from ^{93}Nb and ^{93}Mo.

To address this issue, ion–molecule reactions using H_2 or NH_3 in the reaction cell of inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) have been widely used for Zr isotopic analysis. However, our recent findings indicate that the measured isotopic ratios may be affected by isotopic fractionation during the ion–molecule reactions. Consequently, the observed isotopic ratios of Zr can vary depending on the ion species formed within the reaction cell. Indeed, several previous studies have demonstrated that neither the power law nor the exponential law can be applied to correct mass discrimination effects after ion–molecule reaction processes.

This study investigates the influence of ion–molecule reactions on the mass discrimination effects of individual ion species formed through reactions with NH_3. Figure 1 shows the product ions generated via ion–molecule reactions with NH_3, demonstrating the formation of various species, including deprotonated complexes with coordination numbers ranging from 1 to 6. $[Zr+NH+NH_2+(NH_3)_3]^+$ and $[Zr+NH+(NH_3)_4]^+$ are among the major ion species observed in Fig. 1. The influence of ion–molecule reactions with NH_3 on the measured isotope ratios relative to ^{90}Zr (*i.e.*, $^{m}Zr/^{90}Zr$, where m = 91, 92, 94, and 96) was investigated to evaluate isotopic fractionation in these ion species. The measured isotopic ratio data for Zr exhibited mass independent isotopic fractionation, indicating that careful correction of mass discrimination is essential to derive reliable isotopic abundances of Zr and ^{93}Zr using IDMS with ICP-MS/MS. In this presentation, we also discuss the mechanisms of isotopic fractionation of Zr during collision processes with He compared with ion–molecule reactions involving NH_3.

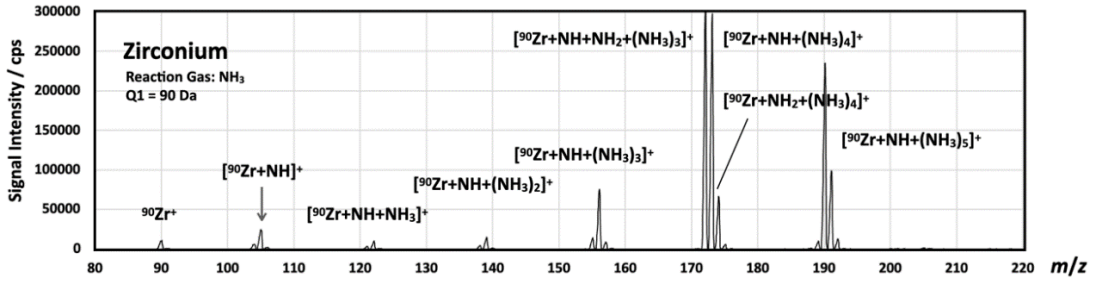

Figure 1 Mass spectrum for Zr obtained through ion reactions with NH_3 using ICP-MS/MS.

This work was conducted as part of a joint study between the Nuclear Regulatory Authority Japan, the University of Tokyo, Gakushuin University, Kyoto University, Institute of Science Tokyo, Japan Atomic Energy Agency, and the National Institutes for Quantum Science and Technology.

(O-7)

Detection of volatile organic compounds through soft ionisation using ICP-tandem mass spectrometry (ICP-MS/MS)

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Inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) is widely used for the sensitive detection of elements. Owing to the high excitation and kinetic temperatures of the ICP, ionization efficiencies exceeding 50% can be achieved for most elements. Although conventional ICP-MS is not suitable for the direct detection of molecules, primarily due to the complete decomposition of organic compounds in the plasma, we recently proposed a novel approach using ICP-MS/MS for the detection of volatile organic compounds (VOCs) via soft ionization based on ion–molecule reactions, such as protonation and cationization.[1,2] In this approach, VOCs are introduced into the collision/reaction cell (CRC) rather than through the ICP ion source, and are ionized via reactions with Ar^+ or various cations (M^+) generated in the ICP. In reactions with $^{40}Ar^+$, the major product ions were protonated ions ($[M+H]^+$), molecular ions (M^+), dehydride ions ($[M–H]^+$), and their fragment ions. Fragmentation induced by electron transfer from analyte molecules to Ar^+ leads to the formation of numerous minor ion peaks in the mass spectra.
In contrast, cationization with $^{107}Ag^+$ produces spectra dominated by silver-adduct ions, represented as $[M+^{107}Ag]^+$. Notably, little to no fragmentation is observed, indicating that cationization with $^{107}Ag^+$ provides significantly softer ionization. To further evaluate the potential of cationization as a soft ionization technique, interactions between VOCs and various metal ions, including Li, Na, Cu, Zn, and Ag, which are commonly used in chemical ionization (CI) and matrix-assisted laser desorption/ionization (MALDI), were investigated. Based on measured cationization efficiencies for three model compounds (benzene, naphthalene, and cyclohexane), several metal ions, including Co, Ni, Cu, Ru, Pd, and Ag, were identified as promising candidates for cationization.[3] The reduced fragmentation enables easier identification of target compounds based on their m/z values.

In this presentation, to demonstrate the practical applicability of the proposed technique, several VOCs released from coffee beans via laser-induced evaporation were monitored. The results highlight the potential of ICP-MS/MS with cationization as a rapid and effective analytical tool for the detection of VOCs in solid samples.

References: (1) Hirata, Kobayashi, Khoo, Shikino, Asanuma (2024) Detection of several volatile organic compounds through Ar^+ induced chemical ionisation using inductively coupled plasma-tandem mass spectrometry (ICP-MS/MS), *Analyst*, 149, 5174 – 5183; (2) Hirata, Kinoshita, Uezono, Khoo (2026) Direct Detection of Volatile Organic Compounds through Cationization Using ICP-MS/MS, *Mass Spectrometry*, 15, 0187; (3) Hirata, Kinoshita (2025) Simultaneous Detection of Elements and Molecules using Laser Ablation-ICP-MS/MS, *Analytical Sciences*, 42, 121–128.

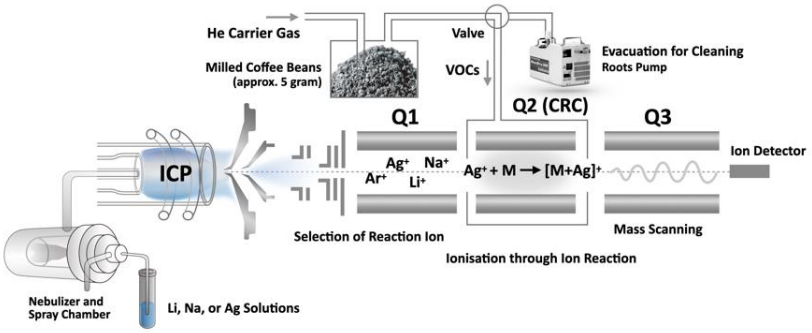

Fig. 1 System setup for the analysis of VOCs in Coffee Beans using ICP-MS/MS

(O-8)

Multi-pressure approach and X-ray desorption of solid reagent precursors for sustainable chemical ionization mass spectrometry

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Chemical ionization mass spectrometry (CIMS) enables sensitive, selective, and continuous detection of environmental trace chemicals, but comprehensive measurements often require multiple reagent ions and instrument configurations, sometimes using hazardous substances. I present two developments toward more practical, low-maintenance CIMS operation without sacrificing analytical performance and extending the range of detectable compounds.

First, multi-pressure CIMS (MPCIMS) combines ambient-pressure ion–molecule chemistry and low-pressure ionization in a single instrument. In α-pinene oxidation experiments, this approach enables quasi-simultaneous detection of compounds ranging from nonpolar volatile organic compounds to highly oxygenated products, reducing the need for parallel instruments. The low-pressure mode shows linear VOC response over two orders of magnitude and only modest humidity sensitivity.

Second, X-ray desorption of solid precursors is introduced as a safe, solid-state route for generating reagent ions. Solid urea is used to produce uronium reagent ions for positive-mode detection of atmospheric bases and other polar compounds, offering high sensitivity, manageable humidity dependence, and long-term stability without maintenance. X-ray irradiation of ammonium nitrate also generates nitrate ions, providing a safer alternative to concentrated nitric acid reagent used in CIMS.

Together, these approaches support safer, simpler, and more deployable CIMS systems. Several real-world applications are demonstrated together with the experimental data.

(O-9)

Optimising ICP-MS analysis: Enhancing helium collision and reaction cell modes

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Inductively Coupled Plasma Mass Spectrometry (ICP-MS) is a key analytical technique for trace elemental analysis. Traditionally, the use of collision/reaction cell (CRC) gases such as helium and oxygen has been somewhat element-specific, requiring detailed method development and frequent gas switching to optimize sensitivity and eliminate interferences.

This study examines the effectiveness of an enhanced single helium mode for analyzing all elements, with the aim of simplifying laboratory workflows without compromising analytical performance. Our results show that operating ICP-MS in enhanced collision mode provides reliable interference removal across a broad suite of elements, including those that are traditionally challenging to analyze. The simplicity of this approach significantly reduces method complexity and the wasted instrument time associated with gas switching, thereby improving efficiency and reproducibility in multi-element analysis.

We are also introducing a new reaction mode in the CRC, offering a sustainable, cost-effective, and safer alternative to bottled oxygen. Experimental data indicate that we can achieve similar levels of interference removal and analytical performance for elements such as sulfur, phosphorus, and arsenic, which typically require oxygen for optimal detection. This further streamlines laboratory operations by eliminating the need for a dedicated oxygen-supply infrastructure.

Together, the enhanced He mode and the new reaction mode can transform routine ICP-MS analysis by optimizing simplicity, safety, and cost-effectiveness, thereby making high-quality elemental analysis more accessible across various laboratory settings.

(O-10)

The Avio 3000: The first third-generation ICP-OES platform built around fundamental redesign

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For several decades, ICP-OES has served as the analytical workhorse in atomic spectroscopy laboratories worldwide. Early instrument generations brought meaningful advances in plasma stability, matrix tolerance, and quasi-simultaneous measurement capability. Progress in recent years, however, has largely centered on incremental refinements to existing platforms or software-level enhancements, leaving core instrument architecture fundamentally unchanged. In 2026, PerkinElmer introduced the Avio 3000 — the first genuinely third-generation ICP-OES — built around a comprehensive and simultaneous redesign of all three core subsystems: plasma generation, optical system, and detection.

At the heart of the Avio 3000 is the innovative HeliPlate™ plasma technology, which builds on the established FlatPlate oscillator design to eliminate the need for an external chiller. This advancement reduces laboratory noise, cost, maintenance burden, and environmental footprint, while enhancing plasma robustness and preserving low argon flow operation. Critically, the HeliPlate™ design enables direct analysis of volatile organic solvents — including 100% methanol — without a chilled spray chamber. Continuous or software-controlled oxygen addition via Syngistix software prevents carbon deposition and maintains plasma stability throughout the analytical run, making the Avio 3000 particularly well-suited for trace impurity determination in demanding organic matrices.

The instrument's custom patented detector, based on a back-side illuminated complementary metal-oxide semiconductor (BSI-CMOS) sensor, delivers full spectral coverage with improved signal-to-noise ratios and measurement precision. These characteristics translate directly to higher sample throughput and enhanced data quality, addressing the productivity demands of modern high-throughput laboratories.

Together, these three foundational innovations represent a substantive departure from the iterative development that has characterized the field for two decades. The Avio 3000 is designed not only to meet today's analytical challenges across a broad range of matrices and applications, but to serve as an extensible platform for continued innovation well into the future.

(O-11)

Fast analysis of environmental samples by ICP-QQQ with discrete sampling

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Environmental laboratories face increasing pressure to boost sample throughput while maintaining high data quality across various matrices, including natural waters, soils, and sediments. These samples often have high levels of dissolved solids and complex interference profiles, making fast and reliable multi-element analysis difficult with traditional ICP-MS methods.
This work describes a high-throughput ICP-MS/MS workflow for routine environmental analysis that combines discrete sampling with advanced interference control using a single helium mode. Helium mode was used as a universal cell condition for most elements, providing effective suppression of plasma- and matrix-derived polyatomic interferences through kinetic energy discrimination and collision-induced dissociation. The use of discrete sampling minimized sample introduction time and reduced exposure of the interface to complex matrices, thereby improving both productivity and long-term stability.

Method performance was assessed using certified reference materials for water, soil, and sediment, along with real-world environmental water samples. Quantitative results showed excellent agreement with certified values, with recoveries typically within ±10%. Limits of quantitation were appropriate for routine environmental monitoring, and more than 140 samples were analyzed in under 2.5 hours, with an average analysis time of less than one minute per sample. Internal standard recoveries remained stable throughout extended analytical sequences, even for samples with high total dissolved solids.

These results show that using a single helium mode combined with discrete sampling allows for fast, accurate, and reliable environmental analysis. The method is ideal for high-throughput laboratories aiming to maximize productivity without sacrificing analytical quality or data integrity.

(O-12)

Innovative multielement analysis strategies for occupational airborne metals: ICP-MS and complementary techniques

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Assessing metal exposures in workplace air remains a central challenge in occupational health, particularly as occupational exposure limits (OELs) for several metals including carcinogenic elements such as Be, Co, Ni, As, and Cd continue to decrease. Target analytes are typically present as particulate matter in fumes and dust, collected on filters as inhalable or respirable particle fractions using portable personal samplers. The limited sampling volumes for personal monitoring (1.2 m^3) and the wide span of OELs and real-world concentrations (ng/m^3 to mg/m^3) impose demanding requirements on analytical sensitivity, calibration strategies, blank control, and measurement uncertainties.

ICP-MS after acid digestion is the standard approach for quantifying airborne metals. However occupational samples differ substantially from ambient aerosols. They combine highly variable and often unknown matrices, trace-level and heterogeneous mass loadings, large concentration spans within a single sampling campaign, as well as matrix- and solubility-controlled preparation limitations. For a contract laboratory with a statutory mandate for prevention, sample preparation and data evaluation are the most time- and resource-intensive steps motivating continuous process optimization to reduce manual work, conserve materials, and maximize reliable information from each sample.

Here we present the continuous optimization of an integrated, routine-compatible workflow for quality-assured ICP-MS determination of 24 analytes, comprising (i) high-throughput single-reaction-chamber microwave digestion optimized for mixed workplace matrices, (ii) procedural blank reduction via purified high-purity acids and blank monitoring, (iii) syringe-driven inline dilution enabling automated preparation of multi-level calibration standards and samples, and (iv) semi-automated data processing to improve efficiency, reproducibility, and data integrity.

To further increase informational yield from a single sample, we present suspension-assisted TXRF as a complementary intermediate step in the ICP-MS sample preparation workflow. TXRF provides rapid multi-element fingerprints and quantitative information of elements and matrix components that are difficult to access by acid digestion, while ICP-MS delivers compliance-relevant ultra-trace quantification and confirmation of critical analytes.

Proof-of-concept results from real workplace samples (e.g. welding/thermal cutting, metal machining, foundries, and battery-related processes) demonstrate how ICP-MS and complementary techniques improve diagnostic value, comparability, and decision-making in occupational safety and health.

(O-13)

Extending the analytical reach of ICP-OES: UV boost mode on the Avio 3000 for the determination of crucial challenging low-UV elements

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ICP-OES is a well-established, rugged technique capable of handling complex matrices with minimal sample preparation, delivering accurate multi-element quantification at ppb concentrations. Despite its broad applicability, a subset of analytically important elements — including arsenic, lead, mercury, phosphorus, selenium, sulfur, chlorine, and thallium — present a persistent challenge. These elements emit weakly in the low ultraviolet region of the spectrum, generally below 220 nm, where detector sensitivity is traditionally limited. As a result, accurate and repeatable measurements at concentrations below 20 ppb are difficult to achieve reliably with conventional ICP-OES instrumentation.

This limitation carries significant practical consequences. Arsenic and selenium are priority environmental and food safety contaminants subject to stringent regulatory limits. Phosphorus and sulfur are critical components in petrochemical, agrochemical, and biological matrices, where low-level quantification is routinely required. Chlorine determination at trace levels is increasingly relevant in materials characterization and environmental monitoring. For all of these elements, the analytical utility of ICP-OES has historically been constrained by the weak emission intensity at their primary — and in many cases secondary — emission wavelengths.

UV Boost mode, an innovative patented feature of the Avio 3000 ICP-OES, directly addresses this limitation by substantially amplifying detector sensitivity below 243 nm. This enhancement enables accurate quantification at lower concentrations in both standard and high-resolution measurement modes, and unlocks the practical use of secondary emission lines that would otherwise lack sufficient intensity for reliable analysis. The result is a meaningful expansion of the analytical dynamic range for low-UV elements, without compromise to instrument robustness or matrix tolerance.

This work presents the performance of UV Boost mode for the analysis of As, P, S, and Cl, demonstrating how this capability elevates ICP-OES as a technique for applications where these elements have traditionally required complementary or alternative instrumentation.

(O-14)

Microplasma ionization coupled to enhanced Orbitrap mass spectrometers: Moving towards elemental and isotopic analysis without chemical separations

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Unfortunately, or fortunately, there is a synergistic, if no co-dependent, relationship between the worlds of separation science and mass spectrometry. Separation methods (e.g., liquid or gas chromatography) do not in themselves provide species identification nor quantification. Likewise, mass spectrometric methods do not generally possess sufficient mass resolution and accuracy to unambiguously provide those same types of information. Very simply, in the case of real world analysis, some form of chemical separation is required prior to many elemental and isotopic determinations. While essential in many instances, solid phase extractions and chromatographic separations add time, cost, complexity, dilution, and the possibility for contamination.

The Marcus group focuses on the development of mass spectrometric strategies that provide chemical and isotopic information across a wide diversity of applications. Specifically, a novel microplasma ionization source, the liquid sampling-atmospheric pressure glow discharge (LS-APGD) has proven valuable in performing elemental, isotopic, and molecular species analysis. With regards to isotope ratio (IR) measurements, the ionization source has been coupled to an ultrahigh resolution ThermoScientific Orbitrap Mass Spectrometer, providing unprecedented mass resolution while delivering precision approaching MC-ICP-MS. Earlier efforts showed that the important geochronological pair of 87Sr and 87Rb could be separated; a mass difference of one beta particle. The microplasma/Orbitrap coupling has been applied for high precision isotope ratio determinations of uranium in the presence of great (>5000x) excesses of problematic elements such as Pb and W; eliminating the need for complex separations prior to IR analysis.

More impressively, we have recently demonstrated the complete isotopic separation of the Nd and Sm isotopes; again allowing for determinations without chemical separations. These measurements are made possible by the implementation of the Spectroswiss FTMS Booster X2, which provides mass resolution in excess of 500,000 on an instrument that is commercially-specified to deliver *only* 70,000, while delivering dynamic ranges that cover up to 7 orders of magnitude as the base system is challenged beyond 4. Limits of detection are on the 10 fg level for most elements. The ultrahigh mass resolution has particular novel opportunities for those cases where extensive chemical separations are required for standard-format elemental mass analyzers including sector-field, multi-collector systems, including cases of direct solid sampling, radioactive samples, and single particle analysis. Recent applications have included direct (no chemistry) determinations of lanthanides and actinides in irradiated, depleted uranium. Additionally, Nd isotope ratios were determined in uranium ore concentrates in the presence of isobaric Sm.

Finally, the capacity to perform high resolution isotope ratio analysis of single-micron CeO_2 particles will be demonstrated. This presentation will provide experimental details of the remarkably simple instrumentation, which holds the promise of performing ***challenging elemental and IR measurements without chromatography.***

(O-15)

Elemental imaging by mass spectrometry at the micro and nanoscale - Challenges and prospects

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Imaging and imaging techniques represent a rapidly expanding domain of major interest within the scientific community. This great success is certainly due to the fact that we humans perceive information much better when it is visualized. Indeed, images facilitate the rapid reception of large amounts of data. In current research, there is a growing interest on integrating structural information with chemical data: specifically, how can we detect chemical elements in each pixel of an image and measure their concentrations? To address this question, a variety of atomic spectrometry techniques are currently employed to chemically map the surfaces of samples within the micro to nanometer scale.

This lecture will highlight important analytical tools for element-specific imaging such as nanoscale secondary ion mass spectrometry (NanoSIMS), laser ablation ICP-MS, and synchrotron-based X-ray absorption spectroscopy. Moreover, the combination of imaging with speciation analysis will be discussed. The application of these techniques covers different scientific fields such as biology, toxicology, nutrition, and geology. This will be illustrated by examples from our current research: mapping and speciation of zinc in zinc-accumulating yeast, assimilation of dietary essential elements by farm animals, as well as isotopic analysis of nanosized particles in bacteria. Furthermore, limitations and new challenges will be discussed, too, along with recent developments towards two- and three-dimensional multimodal, multiscale and correlative imaging.

(O-16)

Understanding the role of ion charge and size in their susceptibility to acoustic ion manipulation (AIM)

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The ability to efficiently gather and control the direction of ionized atoms and molecules is an essential aspect of analytical mass spectrometry (MS) and ion-mobility spectrometry (IMS). Because these analytes are charged, conventional reduced-pressure ion optics utilize electrostatic and/or Lorentz forces to improve throughput from the ionization source to the detector. It is increasingly common for ionization to be performed at atmospheric pressure (AP) due to ease of sample introduction and minimal analyte fragmentation. However, manipulation of ions at AP is difficult due to the short mean free path and the dominance of diffusion. We have recently demonstrated that, surprisingly, all major ions-optic capabilities (i.e. deflection, gating, focusing, and separation) can be achieved at AP with time-varying pressure fields in a phenomenon we refer to as Acoustic Ion Manipulation (AIM). Unfortunately, the initial AIM experiments used small, singly charged, plasma-produced ions (*e.g.*, H_3O^+, N_2^+, etc.) which limited analytical utility and constrained information about the underlying phenomenon.

Here, we describe the coupling of electrospray ionization (ESI) with a standing-wave AIM device to control ions with large differences in size, shape (i.e. conformation), and charge state. In this work, peptide and protein ions were produced from an ESI source and desolvated as they travelled through a heated drying tube prior. The dried ions then passed through a standing acoustic wave formed with two ultrasonic speakers and into a mass spectrometer for detection. Ion beams were deflected away from unstable pressure regions (i.e. antinodes) into the pressure-stable nodal areas. The same AIM optic capabilities shown for plasma-produced ions were found to be possible for large, highly charged biomolecular ions. The use of the drying tube was critical to this process to ensure sufficient desolvation and enable the strongest AIM interaction. Interestingly, a charge-state dependence in the AIM phenomenon was observed where highly charged ions were more greatly influenced by the acoustic field. The behaviors of singly and multiply charged ions traversing a standing acoustic wave were compared and suggest that the electrostatic properties, as well as the resulting higher-order structure, of ions at least partially explain AIM behaviors.

This work expands the capabilities of AIM in the study of biomolecules and reveals novel behaviors of gas-phase ions in the presence of variable pressure fields.

(O-17)

Laser ablation with simultaneous elemental and molecular mass spectrometry imaging: From plant samples to tattoos

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Laser ablation (LA) is one of the most widely used sample introduction methods for inductively coupled plasma-mass spectrometry (ICP-MS), as it allows to directly analyze solid samples without dissolution. While LA-ICP-MS is used since decades for the analysis of geological and materials samples, it has been applied increasingly for the analysis of biomedical samples more recently as well. Due to the high temperatures of the plasma, and thus, its destructive nature, all molecular information is deleted by atomization, while species-independent quantification is enabled.

However, despite the high laser energy at the most widely applied wavelengths of between 193 nm and 266 nm, most molecules remain intact during the ablation procedure. Therefore, when using an appropriate post-ionization procedure as atmospheric pressure chemical ionization (APCI) or related techniques combined with high resolution mass spectrometry (HR-MS), it is possible to obtain spatially resolved molecular information of tissues and other biological samples.

When using a split stream arrangement after laser ablation, it is even possible to simultaneously record elemental and molecular information of the same sample by combining an ICP-MS and an APCI-MS as detectors. Major advantage of this method is the possibility to have a precise spatial alignment of both the molecular and elemental signals.

In this presentation, the general methodology and applications for LA-APCI-MS as well as LA with simultaneous APCI-MS and ICP-MS are presented. These include the analysis of pharmaceutical tablets, forensic samples, tissue samples from tattoos after major complications and plant samples.

(O-18)

Multimodal bioimaging using mass spectrometric and spectroscopic techniques on a single tissue thin section

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The presented study focuses on the development of a workflow to perform multimodal chemical bioimaging on the same tissue thin section. Laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) was used to investigate elemental distributions in pancreatic tumor samples of mice injected with an iodinated and a gadolinium-based contrast agent as well as the chemotherapeutic agent cisplatin. Endogenous elements such as phosphorus, iron and zinc were imaged, as well as the exogenous elements iodine, gadolinium and platinum, which were quantified using matrix-matched gelatin standards.

Other elemental or molecular imaging modalities, including micro X-ray fluorescence (μXRF), infrared (IR) microspectroscopy and matrix-assisted laser desorption/ionization-mass spectrometry (MALDI-MS), were used to validate the results or to obtain complementary information. For a better comparability of images from different modalities, the aim was to perform the analyses on the same tissue thin section. However, this also poses a number of challenges, particularly with regard to the choice of carrier slide and the destructiveness of the different modalities. Different slide materials were compared for the different modalities in terms of signal intensity and background, with indium tin oxide (ITO) slides proving to be most suitable. In addition, for the combination of MALDI-MS and LA-ICP-MS, the additional elemental background caused by the MALDI matrix was investigated as well as the influence of MALDI-MS analysis on signal intensities in subsequent LA-ICP-MS analysis.

(O-19)

Mapping strategies and calibration approaches for laser ablation ICP-MS imaging

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Recent advances in laser ablation ICP-MS imaging have significantly improved spatial resolution, sensitivity, and acquisition speed, enabling increasingly detailed elemental mapping.
In this contribution, practical strategies for setting up LA-ICP-MS imaging experiments will be discussed, with emphasis placed on the advantages and limitations of different mapping parameters such as laser spot size, scan speed, repetition rate, and overlap conditions. Trade-offs and limitations between spatial resolution, sensitivity, analysis time, and image quality will also be evaluated.

Calibration approaches for quantitative imaging will be discussed, including a recently developed volume-corrected strategy in which variations in ablated material are compensated independently of matrix-matched standards. By incorporating separate measurements of ablated volume and applying corrections for laser fluence effects, accurate quantification can be achieved across a wider range of sample types.

Finally, approaches for evaluating image quality and analytical performance in elemental mapping will be discussed, including considerations of limits of measurement (LOM) and just noticeable differences (JND), which may in some applications provide more meaningful metrics than conventional limits of detection (LOD), in context of results obtained by mapping.
Overall, progress toward more robust, quantitative, and broadly applicable calibration and imaging methodologies for LA-ICP-MS will be highlighted.

Analytical Chemistry, 2025, 97, 37, 20108–20116
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Talanta, Volume 269, 1 March 2024, 125379
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(O-20)

Hyphenation of laser ablation with ICP-MS and APCI-MS for simultaneous elemental and molecular imaging of flower buds from the invasive narrow leaved ragwort

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Flower buds from an invasive perennial, the narrow leaved ragwort (*Senecio inaequidens*), are analysed by laser ablation (LA) coupled with inductively coupled plasma-mass spectrometry (ICP-MS) and atmospheric pressure chemical ionisation-mass spectrometry (APCI-MS) for simultaneous elemental and molecular imaging. Longitudinal cryosections were ablated using a laser with a wavelength of 266 nm and a spot size of 20 µm. The resulting aerosol was transported out of the ablation cell with an argon stream and split by a Y-connector, with one part being transported into a single quadrupole ICP-MS for the detection of six elements (^{31}P, ^{25}Mg, ^{44}Ca, ^{55}Mn, ^{63}Cu, ^{66}Zn). The other part was directed to an APCI-Q-ToF-MS with a modified ion source, which allows for the introduction of a dry aerosol, for molecular analysis.

Highest intensities of ^{25}Mg are detected in the phyllaries, where Mg is required for photosynthesis as the central atom of chlorophyll. ^{66}Zn is mostly detected around the ovaries and in the anthers, as Zn is essential for the development of the reproductive system of higher plants, while the ^{63}Cu distribution showed hotspots in the outer sections of the receptacle. Highly localised hotspots of both ^{55}Mn and ^{44}Ca are evident in the tips of the bracts, hinting at a specific accumulation of these elements in these organs. ^{44}Ca is also detected in the stem, where it may aid the structural stability of the stem in the form of calcium oxalate crystals. Using APCI-MS, the distributions of pyrrolizidine alkaloids (PAs), the class of alkaloids mainly responsible for the toxicity of *Senecio* plants, are elucidated. The PAs are located in the anthers of the disk flowers, while the PA-*N*-oxides are located in most tissues, except for the disk flowers. Additionally, nine sesquiterpenoids from two subclasses were detected in the phyllaries and oil cells, where they aid in repelling sucking insects. Furthermore, distinct distributions for di- and triterpenes are observed, which differentiate the anatomical features of the flower bud. The ovaries are distinguished by the presence of the diterpene ion $C_{20}H_{37}^+$, as it is detected only there. The main bodies of the ray and disk flower differ in their terpene profile, as the triterpene ions $C_{29}H_{49}^+$, $C_{29}H_{47}^+$ and $C_{28}H_{47}^+$ are detected in both, while in the ray flower, the triterpene ion $C_{30}H_{49}^+$ is also detected. Apart from the ray flower, this triterpene shows another hotspot in the receptacle. The triterpene $C_{30}H_{47}^+$ is located at the tips of both the ray and disk flowers.

With the capability to spatially resolve endogenous elements, as well as the distributions of both polar and nonpolar molecules, LA-ICP-MS/APCI-MS is demonstrated as a promising tool for the analysis of plants.

(O-21)

Liquid atmospheric pressure MALDI – a multifunctional ionisation technique for biological mass spectrometry

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Liquid atmospheric pressure (LAP)-MALDI represents a transformative convergence of Electrospray Ionization (ESI) and Matrix-Assisted Laser Desorption/Ionization (MALDI), combining the formation of multiply charged ions with the precision of laser-based desorption for high-performance mass spectrometry (MS) analysis. Historically limited to custom-built sources, LAP-MALDI is now fully accessible via commercial high-resolution accurate mass (HRAM) platforms, such as Orbitrap instrumentation. This presentation demonstrates the current breadth of LAP-MALDI applications, highlighting its ability to generate ESI-like data with high signal stability, fmol-level sensitivity, and record-breaking throughput of up to 60 samples per second.

The integration of LAP-MALDI with HRAM mass analyzers facilitates superior proteoform identification and top-down proteomics by resolving overlapping signals that are often indistinguishable in traditional axial-TOF MALDI. Its diagnostic utility through the rapid profiling of microbial species, including Gram-positive/negative bacteria and fungi, will be presented. Beyond simple biotyping, LAP-MALDI enables simultaneous detection of lipids and proteins, coupled with direct MS/MS sequencing from a single sample droplet. Furthermore, the technique's capacity for real-time reaction monitoring and antimicrobial resistance (AMR) testing will be demonstrated. From enzyme kinetics and compound library screening to clinical/veterinary diagnostics and archaeology, LAP-MALDI eliminates traditional analytical constraints, offering a versatile, high-performance solution for the next generation of large-scale and high-speed biological MS analysis.

(O-22)

Rapid evaporative ionization mass spectrometry: From mechanistic insights to subcellular spatial resolution

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Laser ablation Rapid Evaporative Ionisation Mass Spectrometry (LA-REIMS) was originally developed as an analytical technology to monitor cancer surgery interventions using diathermy and surgical lasers. In that regard, REIMS was the first technology which enabled mass spectrometry-guided surgical interventions by providing real-time mass spectrometric information on the tissue being dissected. While the technology in its original form provided information solely on lipid composition and only produced negative ions, the introduction of the so-called ionisation matrix rapidly extended its analytical coverage to metabolites, carbohydrates, peptides and proteins including their positive ions. Following cancer surgery, the technique was successfully applied for clinical microbiology, food safety and animal health applications among others. The technique was also quickly developed into a mass spectrometric imaging platform due to the need for histologically annotated datasets. These datasets are used for building statistical classifiers enabling real-time tissue classification during surgical interventions. While the spatial resolution and sensitivity of the imaging LA-REIMS was limited using standard surgical CO_2 lasers, both parameters showed significant improvement by using short pulse width (nanosecond – picosecond) lasers operating at or close to 2.94 µm. Good beam quality picosecond lasers were found to provide sensitivity and spatial resolution values competitive with commercially available MALDI systems. Data covering murine central nervous system and human cancers will be presented and discussed. Unlike DESI (and to some extent MALDI), LA-REIMS is able to completely ablate the tissue off the support, leaving no residue, enabling a number of experimental approaches including oversampling. Using significant oversampling with a beam diameter of 5-8 µm, <3 µm spatial resolution was achieved, allowing the clear visualisation of cellular nuclei in various tissues. The exhaustive ablation capability also allows the ablation of known amounts of tissue. Since the analyte is not distributed across tissue and matrix layers, this setup – in principle – can also be used for quantitative imaging. Initial attempts to test the linearity of the method will be presented and necessary steps towards global quantitative imaging will be discussed.

(O-23)

Desorption electrospray ionization mass spectrometry: Recent developments for highly sensitive and detailed imaging of biological samples

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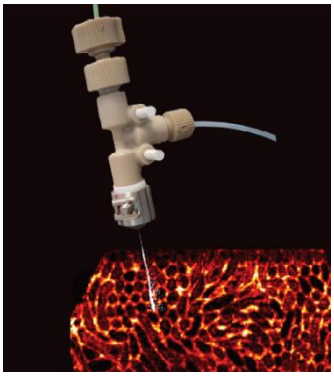
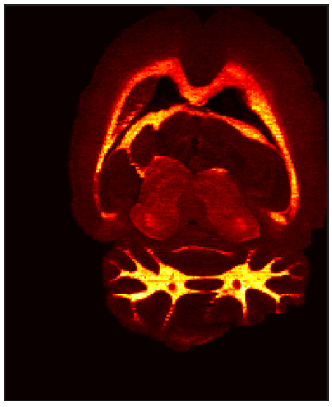
Desorption Electrospray Ionization (DESI) is an ambient ionization technique that enables direct mass spectrometric analysis of solid biological samples under atmospheric conditions. In DESI mass spectrometry imaging (DESI-MSI), charged microdroplets impact the sample surface, extract analytes into a transient solvent film, and generate gas-phase ions through electrospray-like mechanisms, allowing spatially resolved molecular imaging with minimal sample preparation.

This presentation will provide an introduction to DESI-MSI instrumentation and discuss recent developments in DESI technology. Particular focus will be placed on advances in sprayer design, including the introduction of the Desorption Electro-Flow Focusing Ionization (DEFFI) principle and its implementation in the Waters DESI XS high-performance sprayer, as well as a DEFFI sprayer developed in our laboratory for use with Orbitrap mass spectrometers. These sprayer architectures enable improved droplet focusing and dramatically increased ion yield, resulting in significantly enhanced sensitivity and more stable ionization conditions for high-resolution imaging.





The talk will further explore DESI-MSI implemented on triple quadrupole mass spectrometers, where the combination of efficient ambient ionization with multiple reaction monitoring (MRM) enables highly sensitive and selective targeted imaging. The ionization efficiency and analytical performance of DESI in MRM-based imaging workflows will be discussed, with examples demonstrating targeted imaging of pharmaceutical compounds in biological tissues.

In addition to the methodological and instrumental developments, the presentation will include a range of application-driven examples of DESI-MSI. These will illustrate the versatility of the technique across different biomedical contexts, including metabolic profiling of biological tissues, spatially resolved studies of drug distribution and drug delivery, and pharmacological investigations. Together, these examples demonstrate how advances in DESI ionization translate into improved analytical capability for real-world biological and pharmaceutical applications.

(O-24)

Molecules in space and time

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It is a well-known fact that the lipid metabolism and signaling of early stage of pregnancy are of a vital importance in successful embryogenesis. However, the embryo-maternal molecular communication is not well understood, nor it is understood whether the low take home baby outcome of *in vitro* fertilization is the result of some abnormal lipid networking.

The objective of this study was to characterize the spatiotemporal alterations of lipids during the early stage development of natural and transferred mouse embryos. The MALDI measurements were performed in positive reflectron mode in a detection range of m/z 200-3,000. The lateral resolution for MALDI imaging was set to 60 μm or 30 μm. The uterus samples were collected from pregnant animals (natural and transferred embryos) at embryonic day of 4.5, 6.5, 8.5, 10.5, 12.5, respectively. Since phosphatidylcholine (PC) and sphingomyelins (SM) are well ionized in positive mode during MALDI measurements, we were able to identify these subclasses of phospholipids.

Our findings showed significant changes of phospholipid spatiotemporal distribution between the sample cohorts, the phosphatidylcholines as well as the sphingomyelins altered by type and age of pregnancy. Surprisingly, remarkable molecular differences in phospholipids were detected between the identical stage transferred and natural (non-transferred) embryos. On day 6 of normal pregnancy we found an increase for PC 32:0 (16:0/16:0) in uterine stromal cells at implantation sites except for primary decidual zone. In contrast, in transferred animals the PCs showed an increase in glandular epithel at interimplantation sites. On day 8 of normal pregnancy PC 34:2 (16:0/18:2) showed higher level in the antimesometrial pole (AM-pole). In contrast, in transferred uterus samples PC 34:2 (16:0/18:2) were increased in the M-pole. On day 10 of normal pregnancy in the embryonal tissues PC 32:0 (16:0/16:0) and PC 34:0 (16:0/18:0) were increased, while in the AM decidua the two 20:4 containing PCs: PC 36:4 (16:0/20:4) and PC 38:4 (18:0/20:4). In transferred uterus samples higher expression of PC 36:2 (18:0/18:2) in mesometrial decidua was seen, whereas PC 36:4 (16:0/20:4) and PC 38:4 (18:0/20:4) showed increased expression in the AM and lateral decidua. On day 12 of normal pregnancy the SM (16:0/d18:1) was more abundant in the placenta than in case of IVF pregnancy. These molecular differences between the normal and IVF pregnancies can be of a vital importance in successful embryogenesis.

Our results suggest that the embryo transfer induces abnormal phospholipid distribution during the embryogenesis that can be one of the causes of the high rate of failed IVF pregnancies. Further studies are required to discover the embryonic lipid changes during up- and down-regulation of key enzymes of phospholipid pathways.

(O-25)

Direct infusion tools for spatial and cellular METABOLOMICS

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Direct infusion mass spectrometry offers non-labelled and non-targeted analysis of molecules from chemically complex mixtures, such as tissue and cells. However, this material is often precious and limited in volume and concentration, which necessitates innovative mass spectrometry tools for low volume analysis with high sensitivity. Here, I will present our developed tools for direct infusion of cellular extracts - the direct infusion probe, DIP - and mass spectrometry imaging of thin tissue sections with pneumatically assisted nanospray desorption electrospray ionization, PA nano-DESI, in addition to our developed software's for handling the unique acquired data.

(O-26)

Mass spectrometry-based omics sciences for precision medicine and risk assessment of modern therapeutics

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Mass spectrometry-based omics sciences have become a cornerstone of precision medicine, enabling comprehensive and high-resolution characterization of biological systems at the molecular level. By integrating proteomics, metabolomics, and other omics approaches, mass spectrometry provides unparalleled insight into disease mechanisms, patient heterogeneity, and therapeutic response.

This lecture will highlight the application of advanced mass spectrometry techniques in biomedical research, with particular emphasis on their role in the evaluation of modern therapeutics. Special attention will be given to fluorinated drugs, whose increasing use in clinical practice requires sensitive and reliable analytical strategies for the determination of fluorine content, chemical speciation, and metabolic fate in complex biological matrices. These measurements are essential for understanding pharmacokinetics, assessing potential toxicity, and ensuring long-term drug safety.

Proteomics will be presented as a key case study, demonstrating how mass spectrometry-based protein profiling supports the identification of disease-associated pathways and biomarkers. Examples will include inflammatory disorders such as psoriasis, where proteomic analyses reveal alterations in immune signaling, epidermal differentiation, and tissue remodeling. Similar approaches are increasingly applied to other complex diseases, contributing to improved diagnostics, patient stratification, and targeted therapy selection.

Overall, the lecture will emphasize the importance of integrating cutting-edge analytical chemistry with clinical research. Mass spectrometry-driven omics not only advances our understanding of disease biology but also plays a critical role in the development, monitoring, and safety assessment of modern therapeutics, ultimately supporting the implementation of truly personalized medical strategies.

(O-27)

The role of ICP-MS and other MS-techniques in the characterization of biogenic selenium nanoparticles in mushrooms

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Many (micro-)organisms are capable to produce biogenic nanomaterials once exposed to suitable precursors like metal ions. Their production follows a green chemistry strategy generally avoiding hazardous chemicals and harsh experimental conditions. Due to their antibiotic, anti-inflammatory and anti-cancerous activities numerous biogenic nanoparticles (NPs) have attracted great attention for their potential use in medical and pharmaceutical studies.

This presentation intends to give an overview on the characterisation of such biogenic nanoparticles by mass spectrometric techniques. The investigated objects originated from fungi (SeNPs) after incubation with the corresponding precursor ions [1]. Their characterization required several steps: Extraction of the NPs was performed by mechanical lysis of the cells. The nanoparticulate fractions were analysed by single-particle inductively coupled plasma-mass spectrometry (sp-ICP-MS) and transmission electron microscopy (TEM) as complementary tool. This strategy allowed us to characterize the present NPs in terms of shape, size, size distribution and structural composition.

In addition, the natural surface modification (in this case, the protein corona surrounding biogenic Se NPs) was explored by a dedicated combination of an extraction method [2] and liquid chromatography electrospray ionization-tandem mass spectrometry (LC-ESI-MS/MS) [3]. The results revealed the presence of multiple proteins giving hint to the formation and biological pathway of such nanomaterials.

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(O-28)

Analysis of gadolinium-based contrast agent uptake in brain cell cultures using IC-ICP-MS

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Gadolinium-based contrast agents (GBCAs) are used in approximately 40% of clinical magnetic resonance imaging applications to enable more accurate diagnoses. The contrast agents are administered intravenously and then mostly excreted renally in unmetabolized form. In 2006, scientists connected the administration of the linear GBCA gadodiamide to the development of nephrogenic systemic fibrosis in patients with kidney insufficiency. It was assumed that GBCAs were not retained in the bodies of healthy humans. However, in 2014, it was discovered that deposits of gadolinium could be found in brains of healthy individuals.

To investigate the effect of GBCAs on brain cells, an astrocyte cell culture is used. Astrocytes, which are abundant in the brain and serve metabolic, structural, homeostatic and neuroprotective tasks, can provide valuable insights when examined.

The cell cultures are incubated with different linear and macrocyclic GBCAs added into their medium. After incubation, the cells are lysed using a bead mill homogenizer and after filtration, the gadolinium species are analysed. To allow for analysis in the picomolar range an ion chromatography system coupled to an inductively coupled plasma-mass spectrometer is used.

Using this combination, Athmer et al. [1] were able to achieve a separation of six GBCAs within three minutes with limits of detection in the low picomolar range. The chromatographic separation was further optimized for the investigated GBCAs to an analysis time of only two minutes. The speciation results can help to further understand the pathways of GBCAs in the human brain.

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(O-29)

From molecules to elements: Electrospray ionization coupled to high resolution mass spectrometry for trace element speciation

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The distribution of elements between different forms – including isotopic abundances, oxidation states and covalently bound or complexed species – have invariantly been investigated by plasma based techniques, mainly inductively plasma – mass spectrometry (ICPMS), possibly hyphenated to chromatographic separations. As opposite, high resolution mass spectrometry has been traditionally used to investigate, identify, and quantify organic chemical species, prevalently associated with atmospheric pressure ionization techniques like electrospray ionization (ESI). Here we introduce complexation followed by collisional dissociation as key strategies for obtaining elemental speciation information by a conventional ESI source coupled to a high-resolution Orbitrap mass spectrometer. Complexation of elemental ions or species permits their efficient transfer into the gas phase by the ESI source, whereas collisional dissociation before actual mass detection releases the element from the ligand, allowing its detection as a simple singly charged ion.

Two major strategies leveraging these concepts will be presented. Firstly, the definition of a general method for the determination of the isotopic ratios of metal ions will be introduced. The procedure features complexation of the element(s) of interest, introduction into the ESI source followed by collisional dissociation: as a result, the simple, interference free isotopic pattern of the singly charged ion is measured at high resolution. Performances in the case of lead isotopic ratios will be presented. Moreover, the procedure was validated on real-world samples, namely Lake Como sediment specimens, by comparison with multi collector ICPMS data. This represents the first validation of an ESI-MS method for determining lead isotopic ratios in real-world samples.

Secondly, we will present how the same concept may be exploited to determine the environmentally relevant mercury species, namely inorganic and methylmercury, and their isotopic ratios selectively. Here the key idea is employing the soft ionization technique to preserve the molecular information, allowing the separation of inorganic mercury ions and methylmercury by mass spectrometry, provided the species are complexed before introduction into the ESI source.

Applications to samples from the marine food web will be discussed.
Finally, key advantages and constraints, unresolved knowledge gaps and future perspectives will be discussed.

(O-30)

Mercury and selenium isotopic analysis for unraveling Hg detoxification mechanisms in marine biota

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Mercury (Hg) is a is a toxic heavy metal, emitted into the environment as a result of natural processes and anthropogenic human activities. Once released into the atmosphere, Hg undergoes several transformations throughout its complex biogeochemical cycle and finally reaches the ocean. There, it bioaccumulates and biomagnifies in marine biota along the trophic food chain, mainly in one of its toxic forms: Methylmercury (MeHg). As a result, top predatory fish and other seafood species can contain elevated concentrations of MeHg, making the consumption of fish and seafood the primary source of human exposure to MeHg. [1]

Recent studies have shown that Selenium (Se) plays a key role as natural Hg antagonist through the formation of inert Hg-Se nanoparticles. While these interactions have been thoroughly investigated in seabirds and marine mammals, [2-4] uncertainties still remain regarding the role of specific organs in the detoxification process and the internal dynamics of both Hg and, especially, Se in marine fish. [2,5] Our preliminarily study on the determination of the Se isotopic signature in several organs of a Bluefin Tuna fish revealed similar trends between Se and Hg isotopic signatures in the organs analyzed, particularly in the spleen and the kidney. [6] These initial results suggest that combined Se and Hg isotopic analysis may show potential as a powerful approach to further investigate their metabolic pathways in marine fish and to further elucidate the role of Se in Hg detoxification.

Building on these preliminary findings, we are now aiming at a better understanding of Se and Hg interactions in marine fish by exploring another marine species, Atlantic Halibut. In this context, Hg and Se elemental contents, Hg speciation, and dual Hg-Se isotopic signatures were determined across several organs, including liver, kidney, spleen and intestine. By integrating isotope ratio data with elemental speciation, this work aims to contribute to the unraveling of the internal dynamics of Hg and Se in marine organisms and the understanding of the role of Se and specific organs in the detoxification process of Hg.

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(O-31)

Fate of gadolinium-based contrast agents in the body and environment: Insights from speciation studies

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In 2014, repeated administration of linear gadolinium-based contrast agents (GBCAs) was shown to induce signal enhancement in specific brain regions of healthy patients in magnetic resonance (MR) imaging. The unexpected presence of gadolinium (Gd) in the brain challenged the assumption that GBCAs do not cross an intact blood–brain barrier. Although no toxicity has been demonstrated, this retention has drawn increasing regulatory attention. Also, the discharge of the increasing quantities of Gd compounds into the environment raised questions about their transport and fate.

This lecture highlights the synergy of microscopic and mass spectrometric techniques to elucidate the chemical forms of Gd retained in the brain, particularly in deep cerebral nuclei of rats, four months after repeated administration of gadoterate or gadodiamide.[1-3] Gd species were extracted sequentially using water and urea. Total Gd was quantified by ICP-MS, while soluble species were analyzed by size-exclusion chromatography–ICP-MS. Insoluble species were characterized using single-particle ICP-MS, NanoSIMS, and STEM-EDX.

For gadoterate, most Gd was found in the water-soluble fraction, likely as intact GBCA. In contrast, gadodiamide yielded mainly high-molecular-weight (~440 kDa) soluble species with minimal intact complex, suggesting dissociation and formation of labile complexes with endogenous ligands. The majority of Gd, however, was present as insoluble particulate forms. Imaging revealed amorphous, spheroid "sea urchin-like" structures (100–200 nm), with Gd co-localized with calcium, oxygen, and phosphorus, indicating mixed Gd/Ca phosphate phases.

An extension of the study to environmental systems examines the role of nanoplastics as vectors for Gd released into the environment.[4] Using controlled incubation, ultrafiltration, and ICP-MS analysis, the effects of nanoplastic concentration, solution chemistry, and competition with natural colloids were assessed. Notably, up to half of dissolved Gd can adsorb onto nanoplastics even in seawater, with stronger adsorption observed at low nanoplastic concentrations.

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(O-32)

The dark side of ICP-MS: Negative ions for fluorine, PFAS, and beyond

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The determination of fluorine remains one of the last grand challenges in plasma spectrochemistry. Its high ionization potential and inaccessible optical transitions render conventional ICP-based techniques effectively blind to this environmentally critical element. As a consequence, current gold-standard methods such as LC-MS/MS capture only a minor fraction of the total organofluorine burden in environmental and biological samples, leaving a substantial analytical gap in PFAS research.

In this contribution, we present negative ion ICP-MS (nICPMS) as a transformative approach for direct fluorine detection via fluoride ions (F^-), fundamentally extending the capabilities of plasma-based mass spectrometry beyond the traditional positive ion paradigm[1]. We will discuss the underlying plasma chemistry, ion formation mechanisms, and instrumental adaptations required to stabilise and extract negative ions from an inductively coupled plasma.

The analytical potential of this approach is demonstrated across multiple application domains:

i. PFAS analysis beyond molecular selectivity: Element-specific fluorine detection provides access to the total fluorine pool, enabling mass balance approaches and revealing the large unidentified PFAS fraction inaccessible to LC-MS workflows.
ii. Spatially resolved bioimaging: Coupling laser ablation to nICP-MS enables fluorine imaging in biological tissues, exemplified here by the distribution of fluorine in bees, offering new insights into uptake and accumulation pathways.
iii. Single-particle and polymer analysis: Using single-particle ICP-MS (sp-nICP-MS), we extend fluorine detection to particulate and polymeric PFAS, addressing an overlooked environmental compartment.
iv. Speciation concepts: By integrating chromatographic separation with element-specific detection, we explore new avenues for fluorine speciation, bridging the gap between molecular and elemental analytics.

These developments are complemented by alternative ICP-MS/MS strategies (e.g., BaF^+ formation) and emerging plasma concepts, forming a multi-dimensional analytical framework for fluorine determination across dissolved, particulate, and biological matrices.
Overall, this work demonstrates how rethinking ion generation in the plasma - specifically embracing the “dark side” of negative ions - opens fundamentally new analytical windows for PFAS research and challenges long-standing limitations in atomic spectrometry.

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(O-33)

Unravelling the mechanism of glyphosate formation from aminopolyphosphonates by hyphenation of ion chromatography to ICP-MS and ESI-MS

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As the transformation of aminopolyphosphonates (APPs) represents the primary source of glyphosate in the aquatic environment, the identification of further transformation products (TP) and understanding of the underlying transformation mechanism are crucial for environmental assessments. APPs are increasingly used in Europe as detergents, antiscalants and in various applications. After wastewater treatment, they enter the aquatic environment and can be readily transformed by environmental processes. The investigation of the transformation of diethylenetriamine penta(methylenephosphonate) (DTPMP) by ion chromatography (IC) hyphenated with inductively coupled plasma-triple quadrupole-mass spectrometry (ICP-TQ-MS) revealed known but also several unidentified TPs at high fractions. For this reason, a methodology capable of identifying previously unknown TPs by molecular MS and quantifying the TPs species-unspecifically by elemental MS was developed. Hence, the ion chromatographic (IC) separation required optimization for compatibility with electrospray ionisation-mass spectrometry (ESI-MS).

A sodium hydroxide-based eluent system was employed, and after the separation, the column efflux needed to be neutralised by a cation suppressor to achieve volatile conditions. Additionally, a six-port valve was implemented to avoid detector saturation by contaminants. This allowed the separation of seven species standards in 150 s and elemental detection by ICP-MS and molecular detection by ESI-MS in individual runs, while for ESI-MS, zwitterionic species were lost during ion suppression.

With the new methodology, the DTPMP transformation experiment was analysed, and 15 new TPs with proposed structures could be identified by high-resolution MS and fragmentation experiments. This revealed coelution of several species, which could not be distinguished by elemental detection alone. Considering the absolute phosphorus quantification for coeluting TPs as a sum parameter by ICP-MS and the relative feature height of the detected species in molecular MS, the ratios of different TPs could be analysed and gave insight into reaction intermediates and final TPs. The detected TPs confirm the possibility of the formation of a terminal ethyl moiety and its potential oxidation to an aldehyde, which are important steps in previously proposed mechanisms for the formation of glyphosate.

The employed approach combines the advantages of elemental and molecular MS to gain deep insight into the transformation of APPs and their environmental fate.

(O-34)

Examples of trace element speciation analysis in foodstuffs – from research to regulation

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Confidence in the quality and safety of food is a high public priority. The trace elements have their own place in this context with some elements being essential to humans and others harmful. Hence, there is a demand for reliable quantitative information and providing results which are fit-for-the-purpose to enable correct assessment of food quality and/or safety.

Trace element speciation analysis has been among the most important research topics within the field of trace element analysis over the last decades. Food samples are comprised of a high variety of chemical compounds from which many can interact with the elements and form (complex) elemental species with relevance to food quality/safety evaluation. In order to achieve the full picture it is important not only to determine the total amount of a certain trace element present in the food sample but also to identify the chemical form in which given element occurs in given sample (i.e. its speciation).

Selected examples on trace element speciation will be presented with a focus on development and application of methods aiming at control of food safety aspects.

(O-35)

New insights into the speciation of small organically-bound chromium species at low µg kg-1 concentrations in collected aerosols from e-cigarettes using HPLC-ICP-MS

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Accurate and sensitive determination of chromium (Cr) species has crucial importance since the toxicity, bioavailability and transport of this element depend on its chemical form. However, research on Cr speciation has focused so far on the two common free ionic forms, trivalent and hexavalent Cr.

This study reports for the first time methodology for the quantification of small organically-bound chromium species at low µg kg^{-1} concentrations by reverse phase HPLC-ICP-MS. Chromium picolinate (CrP) and chromium acetylacetonate (CrA) were used as model compounds for chromatographic method development and Cr species quantitation. Applying a gradient of aqueous 1,2-hexanediol allowed HPLC-ICP-MS detection of organic Cr species under standard operating conditions without the need for organic-mode set up. The achieved instrumental detection limits were 0.001 and 0.007 µg Cr kg^{-1} for CrP and CrA, respectively, and the measurement RSDs were ≤3.3% for both species (n = 6 at 0.025 µg kg^{-1}).

The developed method was applied to electronic cigarette (EC) aerosols collected on pre-cleaned quartz filter papers under controlled puffing conditions. The sequential extraction and mass balance studies showed that more than 77% of total Cr in the QFPs was water leachable. Speciation analysis of the water fraction revealed that ≥52% of Cr in this fraction was present as small organic species.

An attempt to Cr species identification was undertaken using the developed method with Orbitrap LC-MS detection. Most of the detected Cr species were found stable on the filters and in the aqueous extracts when stored at 4 °C for over 5 weeks. The results described here provide new insights into the chromium chemistry of electronic cigarette aerosols and underscore the importance of chromium speciation for accurate exposure and health-risk assessment in vaping studies.

(O-36)

Laser ablation-based spectroscopy: From multi-elemental tissue mapping to unveiling segregation phenomena in metallurgy

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Laser ablation–based spectroscopic techniques have emerged as powerful tools for spatially resolved, multi-elemental analysis across very different application domains, ranging from biomedical research to advanced materials science. In this work, we highlight the versatility of laser ablation–inductively coupled plasma time-of-flight mass spectrometry (LA-ICP-TOFMS), with special emphasis on ultraviolet femtosecond (UV-fs) ablation, for extracting chemically meaningful information from complex and heterogeneous systems.

On the biomedical side, LA-ICP-TOFMS enables qualitative and quantitative, large-area elemental mapping of thin tissue sections, providing complementary information to conventional histopathology. Applications to cutaneous tumors and liver metastases reveal that pathological processes are accompanied by distinct alterations in elemental composition and spatial distribution. By combining optimized femtosecond ablation conditions with histological imaging, cellular-scale elemental distributions can be achieved while minimizing substrate contributions.

In parallel, the same analytical framework proves highly effective for addressing challenges in metallurgy. Ultra-high-frequency nanosecond laser treatments of Al–Mg alloys induce rapid thermal cycles that promote localized melting and elemental segregation. Subsequent characterization using UV-fs-LA-ICP-TOFMS provides high-resolution, multi-elemental maps of major, minor and trace constituents. While laser-induced surface roughness can degrade signal stability and distort apparent elemental associations, pixel-wise normalization to the total ion signal markedly improves the robustness of correlation matrices. This approach enables a more reliable identification of true segregation phenomena and element-specific interactions driven by laser–matter processes.

References:

Evaluation of femtosecond-LA-ICP-TOFMS for multi-elemental mapping at cellular resolution of human-tissue from cancer patients, J. Pisonero, A. Calon, J. Linares, A. Méndez-Vicente, A. Martínez Nistal, N. Bordel, Optics and Laser Technology, 2025. http://dx.doi.org/10.1016/j.optlastec.2024.111527

(O-37)

Detection and characterization of microplastics by LA-ICP-MS and LIBS

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Microplastics (MPs) are one of the most prominent contaminants in our modern world, having a major impact on all our ecosystems. Several analytical techniques such as FTIR- and Raman Spectroscopy as well as Py-GC-MS or (optical) microscopy are routinely applied to not only detect but also investigate and improve our understanding of the interaction of MPs with the environment. Even though these techniques can provide insights into the number concentration and shape of most MPs, information about the metal profile of MPs is not accessible. Nevertheless, insights into the interaction of metals with MPs is crucial, since MPs are known to act as carriers for other pollutants such as heavy metals. Additionally, some of the above-mentioned techniques have difficulties analyzing environmentally aged MPs with developed biofilm or surface modification as this can alter the spectral signature or cause excessive spectral background signals (fluorescence). Further, one of the most abundant type of MPs, tire wear particles (TWPs), is not detectable at all by FT-IR or Raman spectroscopy due to the presence of carbon black.

In this contribution we present the latest advances of LA-ICP-MS and LIBS for the detection and characterization of MPs, addressing the aforementioned challenges. While LIBS offers the capabilities of laterally resolved polymer classification based on the detection of non-metals (C, H, O, Cl, F,…) and molecular signals (C_2, CN), LA-ICP-MS excels with outstanding sensitivity to investigate the metal profile. The capability of detecting trace metals allows us to investigate the interaction of MPs with heavy metals in prevailing environmental concentrations.

Combining those techniques in a simultaneous LIBS/LA-ICP-MS setup enables the determination of the metal content of individual MPs by applying matrix-matched standards as well as detecting MPs within biological tissues and analyzing the tissues' trace metal profile at the same time. Further, it is demonstrated that LA-ICP-MS alone can be used for laterally resolved polymer classification based on the distinct two-phase sample transport of C for different polymers.

Finally, we present the laterally resolved detection of TWPs in zebrafish guts by LA-ICP-MS using chemometric approaches.

(O-38)

A multi-method platform for the characterization of microplastics: From pristine materials to complex samples

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Over 350 million tons of plastic waste are produced globally every year and are released into the environment at an unprecedented scale [1]. In the environment, larger pieces of plastics are fragmented into microplastics, defined as particles in the size range from 1 µm to 1 mm (according to ISO/TR 21960:2020) or 5 mm (according to Commission Regulation (EU) 2023/2055) and eventually to nanoplastics (with sizes below 100 nm). Microplastics (and nanoplastics) are accumulated in all environmental compartments, including water, soil and air, and are considered critical persistent pollutants of an increasing global concern [2].

Further understanding of the environmental and health implications of microplastic pollution demands for validated analytical methods enabling their detection, "unambiguous" identification, and quantification. Such methods will be invaluable for future risk assessments. However, remaining challenges associated to microplastic analysis arise from the lack of harmonisation of definitions (e.g. measurand definition), the combination of low concentrations of microplastics with matrix complexity often leading to matrix separation/analyte preconcentration workflows to be implemented, the lack of reference test materials (RTMs) needed for instrument calibration, method validation and quality control purposes and the lack of harmonisation of measurement methods needed to support environmental monitoring agencies, testing laboratories and policy makers.

This lecture will firstly demonstrate the potential of a multi-method platform based on the combination of Optical Particle Imaging Analysis (OPIA) and spICP-MS for the accurate determination of number-based concentrations of pristine plastics in the size range of 1-5 µM; with concentration values that agreed well between these techniques for 5 µm PSL particles within their associated relative standard measurement uncertainties (*k=1)* of 11.9% (for spICP-MS) and 2.5% (for OPIA). These led to successful participation in an international inter-laboratory comparison. The lecture will also describe optimisation of laser direct imaging infrared spectroscopy (LD-IR) as a non-destructive technique for the chemical identification and sizing of microplastics with size > 10 µM, assisted by the automated *in house* preparation of microplastic speciated materials (PS and PET mixtures) on a substrate. Such methodology was applied to the analysis of a model food sample (table salt), with results in agreement with those obtained by orthogonal methods based on µFTIR and µRAMAN under the frame of a European Metrology Partnership project (21GRD07 PlasticTrace).

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(O-39)

Development of a multimethod platform based on Laser Direct Infra-Red (LD-IR) imaging spectroscopy for the reliable identification and characterisation of microplastics

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Microplastics, which arise from fragmentation of the plastic waste released into the environment, are accumulated in all environmental compartments at an unprecedented scale and hence are considered critical persistent pollutants of an increasing global concern. [1, 2]. Understanding the environmental and health implications of microplastic pollution requires reliable methods for their detection, identification and characterisation.

This presentation will discuss development of an integrated multimethod platform for the analysis of microplastics, based on the combination of spectroscopy (Laser Direct Imaging Infra-Red Spectroscopy or LD-IR), mass spectrometry (i.e. single particle Inductively Coupled Plasma Mass Spectrometry 'spICP-MS') and imaging optical analysis (i.e. Dynamic Image Analysis 'DIA') techniques, for the reliable characterisation of microplastics within two size ranges (1 – 10 µm) and >10 µm.

Particular attention will be paid to LD-IR as an emerging, non-destructive technique used for chemical identification and characterisation of microplastics of >10 µm. The analytical performance of this technique was verified using two Representative Test Materials (RTMs) of increasing complexity. One of them comprised model spherical polystyrene particles of ~10, 20, 30 and 40 µm characterised with DIA, and another once consisted of polydispersed PET microplastics <500 µm. These were developed and characterised with orthogonal imaging spectroscopy methods under 21GRD07 PlasticTrace project.

A combination of spICP-MS and DIA was found very useful for the characterisation of small microplastics (1-10 µm), with very good agreement achieved for particle number concentration. A good agreement for number concentration was achieved between these techniques for 5 µm polystyrene latex particles. The performance for these techniques for number concentration measurements was demonstrated through participation in an International interlaboratory comparison.

The multimethod platform discussed here represents a promising tool for the characterisation of future Reference Materials and development of harmonised microplastics monitoring in the framework of the emerging legislation (e.g. EU Directive 2020/2184).

[1] H. Ritchie, How much plastic waste ends up in the ocean? OurWorldinData.org, 2018, last accessed 18/09/25.
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(O-40)

Establishing a random forest classifier based on LIBS for process control of galvannealed steel strip

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Industrial galvannealed steel strip production is a continuous, large-scale process where maintaining consistent product quality remains a significant challenge, despite decades of process optimization. Continuous monitoring is indispensable; however, numerous quality control methods rely on offline analyses. This results in a temporal delay between analysis and the ongoing production process, thereby impeding effective process control. For certain applications, the presence or absence of a specific zinc–iron phase - the Zeta phase - as the surface layer is of critical importance, as it substantially influences friction behavior, weldability, and coatability in subsequent manufacturing operations.

This work investigates the feasibility of using laser-induced breakdown spectroscopy (LIBS) as a method to determine the presence of the Zeta phase. LIBS provides elemental information and is already available in portable, hand-held systems and therefore suitable for rapid process feedback. Laboratory-scale LIBS measurements were combined with machine learning to evaluate classification potential. Principal component analysis (PCA) was applied for exploratory data analysis and dimensionality assessment, followed by the development and optimization of a random forest classification model. A structured data-analysis pipeline was implemented to enable systematic model training and evaluation, including comparison of spectral preprocessing strategies such as background subtraction, spectral normalization, and feature reduction through integration of emission bands.

The results demonstrate the methodological basis for rapid, at-line identification of the Zeta phase and provide guidance for transferring LIBS-based monitoring.

(O-41)

How can various ICP-MS techniques provide complementary information on nanogold alterations?

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There is an increasing demand for advanced nanoscale therapeutics, and among these, gold nanoparticles (AuNPs) have proven to afford increased therapeutic efficacy and effective drug delivery. The amount and form in which AuNPs are taken up by cells, the speciation of internalized particles, the routes by which they are translocated inside the cell, and their interactions with subcellular structures can be essential for future approval as anticancer therapeutics. On the other hand, there is an acute need to develop quantitative tools for the effective evaluation of the formation of gold nanoparticle-based anticancer drug delivery systems.

In this contribution, the combined use of ICP-MS-based approaches for the brief characterization of the aforementioned processes will be presented. During the presentation, the potential of direct, single-particle, and hyphenated ICP-MS techniques will be demonstrated for obtaining insights into nanoparticle–cell alterations. Moreover, a brief comparison of electrophoretic versus chromatographic separations with ICP-MS detection for the formation of gold nanoparticle-based anticancer drug delivery systems will be presented. Special attention will be paid to the critical analysis of the optimization step of the methodologies and highlighting their pros and cons.

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(O-42)

Single-particle ICP-MS: New frontiers in uranium particle analysis

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Within nuclear forensics, safeguards, and nonproliferation, the ability to determine actinide content (e.g., U and Pu) and corresponding isotopic abundances (e.g., $^{235}U/^{238}U$, $^{234}U/^{238}U$) across diverse matrices is critical. Detecting these analytes at low abundance within complex matrices presents a classic "needle in a haystack" challenge. While traditional bulk analytical approaches provide high sensitivity, they homogenize heterogeneous particle populations, potentially obscuring particle-specific signatures and leading to misinterpretation of underlying processes. Conversely, particle-focused methods offer higher fidelity but are often labor-intensive and low throughput.

Here, we present an end-to-end, native-particle analytical workflow that preserves uranium particles throughout extraction, introduction, ionization, and detection using single-particle inductively coupled plasma mass spectrometry (sp-ICP-MS). Unlike conventional ICP-MS approaches that rely on extensive digestion and sample preparation, this method maintains particles in their native state, enabling direct, particle-by-particle characterization.

This work highlights recent developments in single particle analysis within nuclear analytical chemistry, with emphasis on the application of multiple ICP-MS platforms, including time-of-flight (TOF), quadrupole, and multi-collector systems, as well as particle-preserving sample introduction strategies. We demonstrate capabilities for particle mass determination, size measurement, and isotopic characterization of uranium particles relevant to safeguards applications.

(O-43)

Calibration approaches for radionuclide measurements ICP-MS/MS

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Operation and decommissioning of nuclear power plants is associated with the need to estimate the radionuclide content in generated waste. Some radionuclides are γ-ray emitters, which are easy to measure using non-destructive techniques and are referred to as easy-to-measure (ETM) radionuclides. At the same time, pure α-, β-, as well as low energy γ-ray emitters, are classified as difficult-to-measure (DTM) radionuclides because they require complex chemical separation and specialised protocols for quantification.

Despite lower external hazards, DTM radionuclides require precise measurement because of their radiotoxicity and long-term health risks. Bioaccumulation can lead to internal exposure and DNA damage. Given their long half-lives, accurate quantification is essential for environmental monitoring, radiation safety, and long-term remediation efforts.

ICP-tandem mass-spectrometry (ICP-MS/MS) is increasingly used as a powerful instrument to address challenges related to the measurement of DTM radionuclides. Due to an additional mass-filter and collision reaction cell, ICP-MS/MS has an enhanced capability for online removal of mass interferences - including polyatomic, tailing and isobaric interferences arising from other radionuclides or stable isotopes - even when the stable isotope concentrations significantly exceed the analyte level. However, the use of this method often requires continuous on-line calibration. This can be problematic due to the limited availability of certified radioactive standards.
To address calibration challenges, several approaches can be implemented. One common method is isotope dilution mass spectrometry, where a known amount of a tracer isotope is added to the sample; the target isotope is then quantified based on the measured isotope ratio.
Secondly, a calibration slope derived from another isotope of the same element can be utilized to facilitate quantification when a direct standard is unavailable.

However, both approaches require mass bias correction, since the detector response and transmission efficiency across different masses are non-uniform. This phenomenon leads to systematic deviations from the true isotope ratio, commonly referred to as mass bias. The mass bias correction typically requires a certified standard isotope mixture of the analyte, however, a mixture of isotopes from a different element can also be used if a reference solution of the analyte is not available and it reacts similar to the analyte.

The third approach is to standardise a solution of the target radionuclide using a calibration slope derived from another element with a similar mass. This is achieved by accounting for mass bias through the measurement of an isotope mixture of a different element, which allows for the accurate interpolation of the instrument's sensitivity at the target mass.

To validate the effectiveness of these approaches, we participated in an interlaboratory comparison for the measurement of several long-lived radionuclides - particularly ^{234}U, ^{235}U, ^{237}Np, ^{239}Pu, ^{240}Pu and ^{241}Am – in the certified reference materials of sea water and silica, as well as ^{93}Mo in stainless steel. The results obtained provide high confidence in our analytical performance and support the continued development of these techniques in future scientific work.

(O-44)

Miniaturized solid-phase extraction – Inductively coupled plasma mass spectrometry (mini-SP-ICP-MS) coupling for U/Pu determination

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Elemental and isotopic determination of radioelements is of primary importance, especially of uranium (U) and plutonium (Pu) which are the major ones coming from the nuclear industry. Their determination is a valuable information for several processes, including spent fuel recycling, waste treatment, monitoring of nuclear facilities, environmental inquiries, and forensic issues.
Direct analysis of U and Pu is extremely challenging in nuclear samples. The latter exhibit high elemental and isotopic complexity, resulting in significant interferences. For example, direct application of techniques such as alpha spectrometry or mass spectrometry is hindered due to multiple radiometric or isobaric interferences, respectively. Solid-phase extraction (SPE), based on commercial particulate resins packed in extraction cartridges, has been widely applied for the chemical separation of U and Pu isobaric interferences, e.g. $^{238}U/^{238}Pu$, prior to mass spectrometric analysis. Despite its high efficiency, SPE is a long process and produces radioactive liquid wastes in the order of several dozens of mL, inducing variable levels of radiation. Moreover, U and Pu determination is carried out in a subsequent step through the analysis of the pure collected fractions.

To this vein, this study presents the development of an analytical approach based on miniaturized SPE coupled to Inductively Coupled Plasma Mass Spectrometry (mini-SPE-ICP-MS) for the online determination of U and Pu from nuclear samples. The proposed alternative involves the *in situ* synthesis of monolithic stationary phases in the channels of microfluidic devices, in order to substantially decrease sample and waste volumes down to the µL level. One of the challenges of this approach is to anchor monolithic phases in thermoplastic materials, chosen owing to their resistance to typical high acidity of the matrices. The online ICP-MS elemental/isotopic determination is further achieved by total introduction of the mobile phase exerted from the microfluidic device, using dedicated total consumption nebulizer associated to a single-pass spray chamber, operating at flow rates lower than 10 µL. min^{-1}.

This communication is focused on the optimization and characterization of an actinide-specific monolithic phase, synthesized in the channels of commercial microfluidic chips. The applicability of this mini-SPE is demonstrated in a conventional laboratory for the elemental separation and the online ICP-MS quantification of ^{238}U and ^{232}Th, used as an analog of Pu. The proposed miniaturized SPE format coupled to ICP-MS through a total consumption sample introduction system would be an important improvement to the conventional approaches, enabling the one-step chemical separation and determination of U and Pu from nuclear samples, while minimizing radioactive liquid wastes.

(O-45)

Isotopic and elemental composition analysis of historical artifacts to enhance the interpretation of past research findings

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The analysis of isotopic ratios and elemental composition is among the key techniques supporting provenance studies of archaeological artifacts (such as bronzes and ceramics) and the reconstruction of the history of artworks. One of the rarely addressed issues in such studies is the representativeness of the results upon which interpretations of an object's features are based. A significant limitation arises from the fact that historical objects, due to their unique and irreplaceable value, cannot be freely sampled - typically, only a single sample can be taken from the entire object.

While non-destructive analysis methods appear ideal in this context, their application is also associated with considerable technical and interpretative limitations. Therefore, it is necessary to develop compromise analytical strategies that, on the one hand, preserve the integrity of the artifact, and on the other, yield reliable and meaningful analytical results.
To date, no studies have systematically assessed the impact of single-point sampling on the reliability of data intended to represent an entire object. In this project, historical artifacts made of bronze and lead were obtained for analysis: fragments of stained-glass window came from the 16th century (18 samples), a bronze axe blade dated to the 1st century BCE (21 samples), and eight samples from a 17th-century Lebanese sarcophagus. Additionally, with the kind cooperation of the National Maritime Museum in Gdańsk, 12 samples were collected from a 17th-century naval cannon recovered from the Swedish galleon Solen, which sank during the Battle of Oliwa in 1627.

All samples underwent microwave-assisted digestion in a closed-vessel system, followed by elemental composition analysis using inductively coupled plasma mass spectrometry (ICP-MS) and lead isotopic ratio composition analysis using multi-collector mass spectrometry (MC-ICP-MS). The results were subjected to a purpose-designed statistical analysis and measurement uncertainty estimation.

The main objective of this study was to evaluate the extent to which a single sampling can provide representative data on isotopic and elemental composition for a given object. The research also aimed to determine the appropriate level of uncertainty that should be associated with such a result in order for it to be considered reliable in representing the entire artifact.

(O-46)

Proton-transfer-reaction mass spectrometry (PTR-MS): Fundamentals and applications in real-time VOC monitoring

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Proton-transfer-reaction mass spectrometry (PTR-MS) is a powerful analytical technique for real-time monitoring of volatile organic compounds (VOCs), combining high sensitivity, rapid time response, and quantitative capability over a wide dynamic range. Modern PTR-MS instruments can achieve limits of quantification down to the parts-per-trillion (ppt) level for many compounds, making the technique highly valuable for trace gas analysis. Over the past two decades, PTR-MS has become widely applied in atmospheric chemistry, environmental monitoring, and emission studies. However, broader routine implementation remains limited in some sectors due to instrumental complexity, data interpretation challenges, and the need for careful method optimization and quality control.

This presentation will provide an overview of PTR-MS, beginning with the fundamental principles of the technique, including chemical ionization via proton transfer, soft ionization behavior, and high temporal resolution measurements. Key operational parameters influencing sensitivity, selectivity, and quantification performance will be discussed. Practical challenges associated with routine operation and data processing will also be addressed. In addition, compound-specific limitations of conventional H_3O^+ PTR-MS measurements will be examined, together with current approaches used to improve chemical selectivity, such as alternative reagent ions and recent methodological developments.

Application examples from our research group will illustrate the capabilities of PTR-MS for real-time atmospheric VOC measurements and emerging applications in airborne tyre-wear particle analysis. Recent advanced PTR-MS hyphenated techniques will also be highlighted, including CHARON for automated online organic sub-micron particle-phase VOC analysis.

(O-47)

Shredding of lithium ion batteries: Investigating material degradation and safety

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Modern state-of-the-art LIBs yet rely on (critical) raw materials such as graphite, cobalt, nickel, and lithium, the development of a closed recycling loop for LIBs is crucial for various reasons: (I) recovery of valuable raw materials, (II) declining abundance of primary resources, (III) environmental concerns associated with mining activities, and (IV) economic and geopolitical risks arising from highly localized supply chains. Moreover, the risk of environmental pollution originating from uncontrolled disposal pathways of toxic battery material is prevented by closed recycling loops for LIBs. The EU regulations specify that 70 wt.% of an LIB must be recycled by the end of 2030 and that specific metal recovery rates of 95% for nickel and cobalt, and 80% for lithium must be achieved by the end of 2031. Equally ambitious targets have been announced by the USA and China

Compared to dry shredding, water-using recycling processes - such as wet crushing and electrohydraulic fragmentation - generate large amounts of contaminated process water, resulting in increased costs for the disposal of hazardous waste and safety guidelines. To improve wastewater management, safety, and sustainability of water-assisted recycling processes, comprehensive knowledge of the battery components in the water are required. Analytical techniques can play an important role during these processes, including all shredding processes and wastewater management.

(O-48)

Correlative imaging workflow combining LA-ICP-MS and IR spectroscopy for gadolinium mapping in neural tissue

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The administration of gadolinium-based contrast agents (GBCAs) in magnetic resonance imaging has been associated with trace-level retention of gadolinium in human tissues. While deposition in the brain has been extensively studied, significantly less is known about accumulation patterns in the peripheral nervous system. This highlights the need for sensitive and spatially resolved analytical techniques capable of quantifying gadolinium distributions in complex biological matrices.

In this work, laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) was employed for quantitative imaging of gadolinium in thin sections of human peripheral nerve tissue. Using a 266 nm laser system, spatially resolved elemental maps were acquired for both transverse and longitudinal sections, enabling detailed investigation of distribution patterns. Matrix-matched gelatin standards were applied for calibration, allowing robust quantification of gadolinium concentrations in the range of 0.05 to 3.1 µg g^{-1}. The data reveal a pronounced accumulation of gadolinium in the perineurium of nerve fascicles, while longitudinal sections indicate a continuous distribution along nerve structures. In addition to gadolinium, endogenous elements such as phosphorus, iron, copper, and zinc were simultaneously monitored, providing complementary structural information and supporting the interpretation of tissue morphology.

To facilitate data interpretation and identification of relevant microstructures, multivariate analysis approaches were applied in combination with complementary molecular imaging by quantum cascade laser (QCL)-based infrared (IR) microspectroscopy. This enabled improved delineation of regions of interest and supported the correlation of elemental distributions with anatomical features.

The presented results demonstrate the capability of LA-ICP-MS for quantitative, spatially resolved analysis of gadolinium in peripheral nerve tissue. The developed approach provides a robust analytical framework for investigating the distribution of metal-based pharmaceuticals in biological systems and contributes to a better understanding of their potential long-term effects.

(O-49)

Advancing fragmentology by multi-technique spectrometric analysis

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Fragmentology is an interdisciplinary field that focuses on detached, reused or dispersed manuscript fragments that are preserved in book bindings from archival or library collections. Through the integration of codicology, palaeography, history, and material analysis, the objective is to reconstruct the origin, dating, and former context of such fragmented written artefacts. Spectrometric and imaging techniques can also be used to investigate selected fragments, providing valuable information on the inks, pigments, and parchment of these manuscript remnants.

A non-invasive analytical approach was applied to investigate unique parchment fragments recovered from the binding of a Hebrew grammar printed in 1600. Historically, protective guards made from reused parchment manuscripts were often sewn into book blocks. Two such guards, attached to the cover of the grammar book, were identified as reused pieces of a Latin psalter containing a continuous Old English gloss. Their attribution to 11th-century England was enabled by comparative historical studies [1].

A comprehensive multi-instrumental strategy was employed to obtain complementary information on the composition, structure, and state of preservation of the fragments. Direct macro-XRF provided non-invasive elemental screening of the written areas, while XRD and Raman spectroscopy enabled phase and molecular identification of pigments and degradation products. Optical coherence tomography (OCT) was used for high-resolution imaging of the parchment microstructure and surface morphology. Additional indirect elemental information was obtained using indicator papers soaked with Bphen and subsequently analysed by LA-ICP-MS for sensitive multielement fingerprinting of transferred species, while MC-ICP-MS measurements delivered high-precision isotopic data where relevant.

Integration of all these complementary datasets enabled detailed characterization of the writing materials and pigments. Particularly informative were the results obtained for the red lead pigment (PbO) present in the rubrication, for which lead isotopic ratios provided additional support for the proposed historical provenance of the fragments.

[1] M. Opalińska, P. Pludra-Żuk, E. Chlebus, *The Eleventh-Century 'N' Psalter from England: New Pieces of the Puzzle*, The Review of English Studies, 2022; hgac081.

(O-50)

Hidden fluorine in gasoline: Multi-technique detection of fluorinated species coming from alkylation processes

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Fluorine-containing species in gasoline samples from different stages of the alkylation process were investigated using multiple analytical techniques, including combustion ion chromatography (CIC), inductively coupled plasma mass spectrometry (ICP-MS/MS), gas chromatography with atomic emission detection (GC-AED), high-resolution continuum source molecular absorption spectrometry (HR-CSMAS), gas chromatography–Orbitrap mass spectrometry (GC-Orbitrap), and 19F nuclear magnetic resonance spectroscopy (19F NMR). This work examines the potential presence of fluorinated compounds in gasoline associated with the alkylation process using complementary analytical techniques targeting both total and molecular fluorine.

Significant variability in fluorine concentrations was observed between samples and analytical methods. CIC measurements indicated total fluorine concentrations ranging from <10 to 321 mg F/L. Comparable trends were observed using HR-CSMAS and ICP-MS/MS. 19F NMR confirmed the presence of several fluorine containing compounds, with the fluorine bound to secondary and/or tertiary carbon. GC-AED analysis further identified volatile fluorinated compounds, reaching up to 269 mg F/L in certain samples, GC–Orbitrap analysis provided high-resolution accurate mass data, allowing molecular formula assignment for the detected compounds.

Overall, the results demonstrate that fluorinated species can occur at various stages of the alkylation process and that combining bulk fluorine determination with molecular-specific techniques provides a more comprehensive understanding of fluorine distribution in refinery streams.

(O-51)

Assessment of metal contamination in cannabis inflorescences and the impact of consumer preparation tools

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Cannabis (*Cannabis sativa L.*) is a widely distributed plant and one of the oldest cultivated species in human history [1]. Despite the growing popularity of cannabis-derived products in recent years, partly due to their potential therapeutic properties [2], cannabis is known to have a high ability to bioaccumulate toxic metals from soil or water [3], which can lead to the presence of undesirable elements in raw materials and finished products. Technological processes associated with cultivation, fertilizing, extraction, and processing of these materials can generate additional contamination and may subsequently find their way into the final product, as reported in previous studies [4].

While contamination from environmental and industrial sources is well recognized, comparatively little attention has been paid to secondary contamination occurring during processing and preparation prior to use. Procedures such as grinding or heating dried plant material may introduce additional metal exposure originating from consumer tools and devices, including grinders and vaporizer chambers made of various materials. Both accumulated metals and secondary contamination may pose risks to consumers and patients.

In this study, we focused on the development of an analytical method for the determination of selected metals (e.g. Pb, Cd, Fe, Cu, Ni) in several cannabis products obtained from diverse sources (online retailers, physical stores, and medical-grade products). We also developed a procedure simulating the grinding of dried plant material by consumers under typical household conditions. This approach was used to evaluate the potential impact of grinders made of different materials (metals, plastics, and ceramics) on the introduction of additional contaminants. For the determination of elements in the ground plant material, samples were subjected to microwave-assisted acid digestion and subsequently analyzed using ICP-MS and ICP-OES techniques.

The findings demonstrate that consumer preparation practices may significantly affect the elemental composition of cannabis products. The observed effects suggest that some grinding devices can influence elemental profiles, while the others seem to be relatively safe to use. This highlights a previously underexplored source of contamination and emphasizes the need for improved quality control not only of cannabis products, but also of consumer tools used during preparation.

[1] R.E. Schultes, A. Hofmann, The Botany and Chemistry of Hallucinogens, Charles C Thomas, Springfield, 1980.
[2] P.F. Whiting et al., JAMA 313 (2015) 2456–2473. https://doi.org/10.1001/jama.2015.6358.
[3] E.E. Golia et al., Sustain. Chem. Pharm. 31 (2023) 100961. https://doi.org/10.1016/j.scp.2022.100961.
[4] D.D. Wright et al., J. Test. Eval. 52 (2024) 3221–3231. https://doi.org/10.1520/JTE20230621.

13 Short Course Abstracts

(A-1)

Tracing nanomaterials in biological systems: A brief overview on sample preparation and characterisation techniques

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The analysis of nanomaterials has become a very important challenge in the environment and biological systems. Their increasing industrial production and their impact on our daily life has raised concerns about the potential effects on living organisms.

The study of such effects requires analytical methodologies that permit an unambiguous and representative 'picture' of the nanomaterials present in the biological system. This starts from a dedicated sample preparation strategy, e.g. to extract the analytes from the matrix, followed by using suitable characterization techniques.

This short course intends to give an overview on existing extraction methods suitable for nanomaterials present in biological samples: chemical, enzymatic, and mechanical approaches will be critically discussed.

The second part will focus on current characterization methods with emphasis on tools implementing inductively coupled plasma-mass spectrometry (ICP-MS). Basics on single particle ICP-MS as well as hyphenated techniques with ICP-MS as detector will be presented on some selected examples including nanomaterials containing elements like Au, Ag, Fe, and Se.

(A-2)

An introduction to machine learning for sample classification based on elemental fingerprinting

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Combining elemental analysis with multivariate statistics and machine learning methods enables powerful strategies for sample classification and discrimination, often referred to as elemental fingerprinting. These techniques support the development of robust and reliable classification models and are widely applicable across diverse fields, including forensics, geology, food authentication, and environmental analysis.

This short course provides an intuitive, practice-oriented introduction to commonly used supervised and unsupervised machine learning algorithms. Rather than focusing on mathematical formalism, the course emphasizes conceptual understanding and practical application.

Participants will gain insight into the fundamental principles of these methods, as well as their strengths, limitations, and common pitfalls when applied to elemental datasets. Particular attention is given to appropriate model evaluation and performance assessment to avoid overfitting. An interactive Python-based example is included to demonstrate a typical workflow, from data preprocessing to model development and interpretation of results.

(A-3)

Development and applications of ion sources in biological MS

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This short course will focus on the practical aspects of the development, refinements and (lab-) environmental aspects for ion sources made to facilitate biological mass spectrometry and its specific applications. It will touch on aspects that are rarely discussed in the literature such as the lab's relative humidity as well as the ultimate analytical utility of specific ion sources with a view on sensitivity, versatility and applicability to various analytes and analytical questions. It will try to provide a comparative understanding about the pros and cons of a range of ion sources in the jungle of modern ion source developments in biological mass spectrometry, in particular where lasers are utilized for sample ablation to initiate the desorption/ionization process.

We will conclude with an interactive discussion on questions and ideas regarding this field – a topic largely overlooked by both commercial manufacturers and academic research groups.

(A-4)

Nuclear material characterization: Tools, techniques, and emerging capabilities

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Accurate characterization of nuclear materials is essential for nuclear fuel cycle development, safeguards, nonproliferation, advanced reactor deployment, waste management, and forensic investigations. This short course provides an overview of modern analytical approaches used to determine the elemental and isotopic composition of nuclear materials, with a primary emphasis on inductively coupled plasma optical emission spectroscopy (ICP-OES) and inductively coupled plasma mass spectrometry (ICP-MS). Participants will gain foundational knowledge of the principles, instrumentation, sample preparation strategies, calibration approaches, and data interpretation methods associated with these powerful techniques.

The course will explore how ICP-OES and ICP-MS are applied to the characterization of nuclear materials, including discussion of trace elemental analysis, impurity quantification, isotopic ratio measurements, and ultra-low-level detection capabilities. Practical considerations such as radiological sample handling, matrix effects, interferences, quality assurance, and uncertainty evaluation will also be addressed. In addition, the course will highlight recent advances and emerging capabilities in nuclear analytical science, including high-resolution and multi-collector ICP-MS, laser ablation methods, automated sample introduction systems, and integration with complementary characterization techniques.

Designed for scientists, engineers, students, and technical professionals working in nuclear science and engineering, this course combines theoretical background with real-world application examples to provide attendees with a practical understanding of current and next-generation nuclear material characterization capabilities.

(A-5)

An introduction to isotop analysis using single- and multi-collector ICP-MS

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In contrast to most analytical techniques for trace element determination, ICP-mass spectrometry (ICP-MS) also provides access to isotopic information. Many ICP-MS users already exploit this feature when assessing the potential occurrence of spectral overlap by comparing measured and theoretical isotopic patterns or by applying mathematical interference corrections. Beyond these routine applications, however, isotopic analysis enables a much broader range of powerful analytical approaches.

Measuring *induced* changes in isotopic composition allows the application of isotope dilution as a highly robust and reliable quantification strategy, while similar concepts underpin tracer experiments used, for example, to study the uptake of essential mineral elements from food.
In addition, elements with radiogenic isotopes (such as Sr and Pb) exhibit pronounced natural isotopic variability, which can be exploited for geological dating and provenance studies of the raw materials used to manufacture archaeological artifacts, agricultural products, and human remains.

While single-collector ICP-MS may suffice for basic isotope ratio measurements, the detection and quantification of differences in isotope ratios resulting from natural isotope fractionation effects generally requires the higher precision offered by multi-collector ICP-MS (MC-ICP-MS). MC-ICP-MS has therefore become a powerful tool in fields such as geo- and cosmochemistry, environmental sciences, and biomedicine.

This short course will briefly cover the theoretical background underlying natural variations in isotopic composition, provide practical guidance on isotope ratio measurements using ICP-MS, and highlight best practices and common pitfalls. The added value of isotopic analysis in addressing real-life problems will be illustrated using applications from the author's laboratory and/or reported in the literature.

(B-1)

Workshop on laser ablation-ICP-mass spectrometry

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Laser Ablation-Inductively Coupled Plasma Mass Spectrometry has been introduced in 1985 by Alan Gray [1]. Since that time a lot of fundamental studies have been carried out, which include the ablation process, the selection of wavelength, the influence of the ablation chamber and the aerosol transport system as well as the ICP-MS parameters influencing the accuracy of direct solid analyses. Furthermore, methods to determine the transport efficiency and the role of the carrier gas will be discussed in great detail.

Currently, more than 1100 manuscripts are currently published per year using this direct solid analysis technique. However, some of the applications are purely qualitative and include image generation of a wide variety of objects. Therefore, the workshop will cover most important methodological developments to provide quantitative data using LA-ICP-MS. Some selected applications using a variety of ICP-MS instruments will be discussed.

[1] A. Gray, Solid Sample Introduction by Laser Ablation for Inductively Coupled Plasma Source Mass Spectrometry, Analyst 1985 Vol. 110, 551

(B-2)
Practical approaches to the use of reaction gases in triple quadrupole ICP-MS

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Unlock the full potential of your ICP-MS/MS. This short course offers an application-focused approach to method development, designed for users who want to move beyond routine operation and gain real control over reaction cell chemistry.

Through clear explanations and practical examples, participants will learn how to confidently select and manipulate reaction gases to overcome complex spectral interferences. The course demystifies ion–molecule reactions and shows how to turn them into powerful analytical tools.

Key questions we will tackle include:

- Does the analyte or interfering species react exothermically or endothermically with a given gas?
- How does collision energy influence reaction pathways and efficiency?
- Why does ionization energy matter when choosing reaction conditions?
- Which gases are best suited for specific analytes and interferences—and what product ions are formed?
- Which cell parameters are most critical during manual optimization, and how can they be tuned for maximum performance?

Using real-world examples of polyatomic, doubly charged, and isobaric interferences, this course provides practical strategies that can be immediately applied in your own laboratory.
Whether you are troubleshooting challenging analyses or aiming to push detection limits, this course will equip you with the insight and confidence to master ICP-MS/MS reaction chemistry.

(B-3)

Metrological and standardisation advances for particle concentration: From inorganic nanomaterials to bio-nanoparticles to microplastics

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This short course will illustrate how some of the analytical challenges related to the characterization of *i*) nanomaterials, including engineered inorganic nanomaterials and those used in drug delivery systems/nanomedicines and *ii*) microplastics in pristine materials and food-related samples have been overcome through a variety of practical examples in which platforms including the combination of asymmetrical field-flow-fractionation (AF4) with light scattering/ICP-MS, Optical Particle Imaging Analysis, Laser Direct Imaging Infrared Spectroscopy (LD-IR) and spICP-MS play a key role.

It will also highlight remaining analytical challenges driven by legislation, existing reference materials and documentary standards as well as the importance of interlaboratory comparisons to assess the state-of-the-art of measurements performed by expert laboratories.

(B-4)

Secondary ion mass spectrometry for elemental and isotopic imaging

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In this short course, element specific imaging techniques with a focus on secondary ion mass spectrometry (SIMS) will be presented. In a first part, the principles of SIMS including ion sources and the ionization process will be covered as well as the difference between dynamic and static SIMS techniques. This course discusses also briefly related X-ray based techniques such as electron microscopy with energy-dispersive X-ray spectroscopy (SEM-EDS, TEM-EDS, synchrotron radiation XRF). Specifications and limitations regarding spatial resolution and sensitivity will be discussed.

The second part will focus on nanoscale secondary ion mass spectrometry (NanoSIMS) for chemical and isotopic imaging at the submicrometer scale: principle, ion sources, ion transmission, lateral resolution, mass resolution, and useful yield. This course discusses furthermore challenges of sample preparation especially for biological material as well as solutions for correlative imaging with related techniques. Applications from our work on plant and animal tissue, cell cultures as well as geological samples will be presented in order to illustrate and discuss challenges and limitations of the (Nano)SIMS technique. Finally, in the last part, solutions for the treatment of imaging data and their limitations will be presented.

(B-5)

Ambient ionisation mass spectrometry

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The short course will cover the fundamentals of ambient ionisation, including the main principles of ionisation. Ionisation scenarios involving charged droplets, chemical ionisation and de-coupled sampling/ionisation will be discussed together with the ion energetic aspects of the various processes.

The fundamentals session will be followed by a session on true ambient applications, where mass spectrometry is deployed outside of the laboratory to analyse samples in their native, ambient environment. Applications in interventional medicine, animal health, food safety, transportation security and forensics will be discussed.

The third session will focus on the application of ambient ionisation in high throughput analytics. Fields of applications ranging from industrial quality control through clinical chemistry to food analysis will be discussed together with the corresponding sample management and mass spectrometric instrumentation concepts.

The last session will cover the mass spectrometric imaging applications of ambient MS. Spatial analysis using Desorption Electrospray Ionisation (DESI), nanoDESI and Rapid Evaporative Ionisation Mass Spectrometry (REIMS) will be discussed in detail. Ion source setups and corresponding limitations will be reviewed in the context of applications.

(C-1)

Introduction to GD-MS for direct analysis of innovative materials

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The continuous development of innovative materials in modern manufacturing, such as thin-film photovoltaic devices, high wear-resistant coatings, magnetic storage media, and Ni- and Co-based superalloys, demands analytical techniques capable of providing fast, reliable and quantitative elemental information directly from solid samples. In this context, glow discharge mass spectrometry (GD-MS) has emerged as a powerful and mature methodology for the direct analysis of bulk materials and layered structures, offering a valuable complement to more established surface-sensitive techniques.

This introductory course presents the fundamental principles and analytical capabilities of GD-MS, with emphasis on its suitability for the characterization of advanced materials. After a brief historical overview of glow discharge ion sources and their coupling to modern mass analysers, the basic operating concepts of low-pressure glow discharges are discussed, including sputtering processes, plasma formation and the temporal and spatial separation between sample erosion and ionization. Attention is given to the main ionization mechanisms involved in GD-MS, electron ionization, asymmetric charge transfer and Penning ionization, and their impact on sensitivity, selectivity and matrix effects.

The course further addresses practical aspects relevant to real-world applications, such as the differences between DC, RF and pulsed glow discharge operation modes, and their respective advantages for the analysis of conductive and non-conductive materials. The capability of GD-MS to perform rapid depth profiling with smooth sputtering rates, low thermal load and reduced matrix effects is highlighted, illustrating its usefulness for the characterization of coatings, multilayers and functional surfaces. In addition, the potential of pulsed and RF glow discharge sources as complementary tools and even as sample preparation platforms for other surface-analysis techniques is introduced.

Overall, this course aims to provide participants with a clear and intuitive understanding of how GD-MS works, what type of analytical information it can deliver, and where its strengths and limitations lie.

Glow Discharge Mass Spectrometry, Cristina Gonzalez-Gago, Nerea Bordel, and Jorge Pisonero, University of Oviedo, ASM Handbook, Volume 10, Materials Characterization, ASM Handbook Committee, 2019, DOI 10.31399/asm.hb.v10.a0006648.

(C-2)

Fluorine and PFAS analysis – Linking molecular and elemental detection

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Building on the preceding lecture on negative ion ICPMS[2], this workshop focuses on practical analytical strategies to close the fluorine mass balance in PFAS analysis. Within the context of evolving EU regulations and group restrictions, participants will first revisit the basics of PFAS analysis by LC–MS/MS and LC–HRMS, including targeted quantification, non-target screening, and their inherent limitations in capturing the total organofluorine burden.
The workshop then introduces sum parameters (EOF/AOF and total fluorine) and their growing regulatory relevance. A central theme is how to bridge the gap between molecular and elemental information, using ICP-based techniques as compound-independent detectors.
Particular emphasis is placed on the BaF^+ method in ICP-MS/MS[1], demonstrating how conventional ICP-MS instruments can be adapted for fluorine detection, including calibration strategies and analytical constraints. In addition, participants will learn how to perform speciation analysis with ICP-MS, combining chromatographic separation (e.g., HPLC-ICP-MS) with element-specific detection to quantify known and unknown PFAS independently of molecular standards.
Through case studies and interactive discussion, the workshop provides guidance on mass-balance evaluation, method selection, and identification of analytical blind spots, enabling participants to move beyond routine workflows toward integrated, regulation-relevant PFAS analytics.

1. Jamari, N.L.A. et al. *J. Anal. At. Spectrom.* **2017**, 32, 942–950.
2. Raab, A. et al. *J. Anal. At. Spectrom.* **2025**, 40, 1689–1699.
3. Müller, V. et al. *J. Anal. At. Spectrom.* **2025**, 40, 1700–1710.
4. Al Zbedy, A. et al. *Anal. Chim. Acta* **2025**, 1351, 343855.

(C-3)

Laser ablation and molecular mass spectrometry: Fundamentals and applications

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Imaging mass spectrometry of molecules most frequently is applied based on matrix-assisted laser desorption/ionization mass spectrometry (MALDI-MS), desorption electrospray ionization (DESI)-MS or secondary ion mass spectrometry (SIMS). However, in the field of elemental mass spectrometric imaging, laser ablation-inductively coupled plasma (ICP)-MS is the most established method for the analysis of a wide range of samples.

While LA-ICP-MS is destructive due to atomization of all molecules in the plasma, the laser ablation process itself is more gentle towards the sample constituents than frequently assumed. Combining LA and suitable postionization mass spectrometric methods as atmospheric pressure chemical ionization (APCI)-MS or dielectric barrier discharge ionization (DBDI)-MS does therefore allow to observe intact molecules under certain precautions.

Therefore, the addition of a laser ablation system allows to use any commercial atmospheric pressure ionization mass spectrometer for molecular imaging after only very minor technical modifications.

Labile analytes, however, may suffer from thermal effects, as can be seen when testing the method in comparison of dried analyte droplets and analytes embedded in gelatin. While the latter show very limited fragmentation, the former are more likely to be fragmented, probably due to limited heat dissipation and thus, increased thermal effects on the analytes. While this has to be considered when interpreting mass spectra of complex samples, it also offers additional analytical possibilities. Among these are the observation of carbohydrate fragments from starch after depolymerization and dehydration in plant samples and the option to use LA-APCI-MS for the analysis of polymers based on targeted fragmentation caused by thermal effects. In this case, mass spectra are characteristic for different polymer classes and resemble those of pyrolysis-gas chromatography (GC)-MS.

In this short course, fundamentals of molecular postionization-MS after LA and several applications from different fields of research are presented.

(C-4)

Matrix-assisted laser desorption/ionization (MALDI)-MS: A powerful mass spectrometry imaging technique

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Matrix-Assisted Laser Desorption/Ionization Mass Spectrometry Imaging (MALDI-MSI) is a transformative, label-free analytical technique that bridges the traditional gap between mass spectrometry and histopathology. By enabling the direct visualization of molecular distributions—including proteins, lipids, and metabolites—within intact tissue sections, it provides a "molecular histology" that reveals phenotypic heterogeneities often invisible under conventional microscopy.

The workflow begins with the preparation of fresh-frozen or formalin-fixed paraffin-embedded (FFPE) specimens sectioned onto conductive Indium-Tin-Oxide (ITO) slides. A chemical matrix is applied via automated spraying or sublimation; for protein-focused discovery, Sinapinic Acid (SA) is often utilized, while DHB is preferred for lipids and CHCA for high-resolution peptide mapping. Laser ablation across a predefined raster induces desorption and ionization, specifically targeting the 2,500–25,000 range for clinical proteomic signatures. Digital H&E co-registration ensures that mass spectra are precisely mapped to morphological structures.

MALDI-MSI offers high clinical utility for risk stratification and the identification of therapeutic targets. By resolving "histologically invisible" tumor subclones, this technology facilitates the development of personalized therapy through a refined, molecular understanding of the tumor microenvironment.

(D-1)

Plasma source mass spectrometry for trace element speciation analysis: From principles to practice

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Trace element speciation analysis is essential for understanding the role of metals and metalloids in environmental, biological, and clinical systems. While total elemental concentrations provide limited information, it is the specific chemical forms that determine mobility, bioavailability, and toxicity. This short course introduces the fundamental principles of speciation analysis and explains why distinguishing between species is critical.

The course begins by addressing key analytical challenges, including ultra-trace sensitivity, species-specific detection, reliable identification, and accurate quantification. These challenges define the requirements for analytical methodologies and drive the development of advanced instrumental approaches capable of handling complex matrices.

A central focus is plasma source mass spectrometry, particularly inductively coupled plasma mass spectrometry (ICP-MS), as a powerful element-specific detector. Its high sensitivity, wide dynamic range, and near-species-independent response make it especially suitable for quantitative speciation when coupled with separation techniques. The principles and role of ICP-MS in speciation workflows are introduced.

The integration of ICP-MS with separation methods such as gas chromatography, liquid chromatography, and capillary electrophoresis is then examined. These hyphenated techniques enable the resolution of complex mixtures into individual species prior to detection, significantly improving analytical specificity while introducing practical challenges in method development.

Since ICP-MS provides no structural information, its complementarity with molecular mass spectrometry, particularly electrospray ionization mass spectrometry (ESI-MS), is discussed. Combining elemental and molecular detection enables both quantification and structural characterization of metal-containing species.

Finally, modern workflows and selected case studies illustrate the application of integrated strategies in metallomics and environmental analysis. Emphasis is placed on practical aspects such as species stability, method validation, and data interpretation, highlighting future trends in the integration of atomic and molecular mass spectrometry.

Basic readings:

J. Szpunar and R. Lobinski, *Hyphenated techniques in speciation analysis* (2003) Royal Society of Chemistry, Cambridge, UK.

S. Mounicou, J. Szpunar, R. Lobinski, *Metallomics: the concept and methodology*, Chemical Society Reviews (2009) **38**,1119-1138.

(D-2)

Orbitrap mass analyzers for elemental and isotopic analysis

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Perhaps the greatest of advance in the area of biological molecule mass spectrometry has been the advent of the orbitrap mass analyzer. Orbitrap mass spectrometers provide the ultimate in obtainable mass resolution, with commercial off-the-shelf (COTS) systems providing $m/\Delta m$ = 70,000 – 1,000,000. While a scarcely studied aspect of the instruments, the fact that ion packets are captured and processed in a simultaneous fashion should also provide greater measurement precision for isotope ratio (IR) analysis.

The laboratory of Marcus et al. have coupled the liquid sampling-atmospheric pressure glow discharge (LS-APGD) microplasma to a variety of orbitrap platforms, concentrating of methods development of uranium IR measurements. These efforts have been paralleled by efforts by the group of Shelley using a solution cathode glow discharge (SCGD) Eiler who has concentrated on IR measurements for GC/MS analysis of small organic molecules. There had been efforts in coupling ICP sources to orbitraps, but nothing has been presented in the open literature. As the commercial Orbitrap systems were designed for a diverse array of "organic MS" applications, they do not share the measurement goals necessary for elemental and isotopic analysis, most specifically the quantitative aspects. These measurements are made possible by the implementation of the Spectroswiss FTMS Booster X2T, a third-party data acquisition/processing unit that operates in parallel to the base instrument's detection electronics. By use of an absorption mode FT processing, true background sigal characteristics can be accessed to provide better overall sensitivity. Likewise, the ability to process thousands of spectral co-ads provides ultimate S/N improvement, ultimately delivering dynamic ranges that cover up to 7 orders of magnitude as the base system is challenged beyond 4. Finally, use of the Booster system mass resolution in excess of 500,000 on an instrument that is commercially-specified to deliver *only* 70,000. We present here the rationale and experimental variables which have been evaluated towards obtaining high precision IR measurements.

Specific examples will concentrate on the uranium isotopic system, which itself is challenging due to the wide dynamic range. Interlaboratory comparisons involving TIMS and SF-ICP-MS will be presented. Use of novel data acquisition systems and alternative processing methods will be presented as paths forward to obtaining high resolution, high precision IR analysis.

(D-3)

LA-ICP-MS mapping: from fundamentals to high resolution calibrated elemental maps

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This short course will cover the fundamentals of LA-ICP-MS mapping and provide practical insights into optimizing parameters to achieve the highest possible image quality. Before adjusting acquisition settings, it is essential to understand the instrumentation currently in use, along with its strengths, limitations, and best practices for effective operation.

In addition to key experimental parameters such as laser fluence, beam size, and repetition rate, the course will explore calibration strategies and different quantification approaches, including a discussion of their advantages and limitations.

By understanding how these factors interact, participants will be better prepared to design and carry out experiments confidently, resulting in high-quality quantified elemental maps.

(D-4)

Direct analysis mass spectrometry with atmospheric pressure plasmas

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Electrical plasmas and mass spectrometry (MS) have gone hand-in-hand since J.J. Thomson used a reduced-pressure glow discharge as the first ionization approach in the discovery/development of mass spectrometry. Historically, plasma ion sources were used for these experiments because they were one of the few known sources of gas-phase ions at the time and they were relatively simple to setup and operate. However, developments in plasma ionization have continued to inform and motivate advances in other areas of MS long after the work of Thomson and Aston. More recently, atmospheric-pressure (AP) plasmas have been explored for a variety of purposes including direct mass-spectrometric analyses, molecular and elemental ionization, surface modification, chemical synthesis, and environmental remediation.

Atmospheric-pressure discharges are unique in that they simultaneously produce highly energetic species as well as lower energy chemical reagents. Furthermore, it has been shown that plasma conditions (e.g., power, gas composition, etc.) can be slightly altered to favor one condition, even on the timescale of analysis.

This short course will cover emerging trends in AP plasma source usage in chemical and analytical sciences, with an emphasis on methods that utilize MS.

(E-1)

Analytical characterization of nanomaterials

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This short course provides an overview of modern analytical strategies for characterizing nanomaterials, emphasizing both elemental and surface analysis. Participants will gain an understanding of the underlying physical principles, instrumental approaches, and data interpretation methods required to probe the size, morphology, chemical composition, and surface characteristics of materials at the nanoscale. The session integrates practical insights from state-of-the-art instrumentation and real-world applications in environmental science, materials engineering, and nanotechnology.

Segment 1: Synthesis and applications of nanomaterials

- Definition and classification of nanomaterials
- Overview of key synthesis strategies and their analytical challenges
- Importance of advanced characterization in quality control, performance optimization, and regulatory contexts

Segment 2: Analytical requirements and sample considerations

- Fundamental analytical challenges unique to nanoscale systems: agglomeration, dissolution, and matrix effects
- Sampling, sample preparation, and contamination control
- Comparative overview of major analytical techniques used for nanoparticle characterization

Segment 3: Single-particle elemental and isotopic analysis

- Principles of plasma-based analytical tools bulk and trace composition
- Introduction to single-particle analysis for size and number concentration determination
- Application of mass spectrometry for isotopic and elemental fingerprinting
- Case examples from environmental monitoring and engineered nanoparticle analysis

Segment 4: Surface and depth profiling techniques

- Fundamentals of surface-sensitive methods
- Surface composition, isotopic mapping, and depth profiling in complex nanostructures
- Comparison of analytical performance and spatial resolution across methodologies

Segment 5: Data integration and emerging frontiers

- Hyphenated and correlative approaches
- Data quality, validation, and uncertainty assessment
- Advances in real-time, high-resolution, and AI-assisted nanoparticle characterization
- Concluding discussion on analytical innovation and its role in nanomaterial design and policy

14 Poster Abstracts

(P-1)

Development of a certified water reference material to support laboratory measurement traceability

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The project aims to develop a detailed strategy for producing a certified reference material (CRM) based on natural water enriched with selected elements and ions, named Multifunctional Polish Natural Waters (MPWN). It is intended to support the national metrological system by improving the availability of regionally relevant CRMs for environmental monitoring and applications such as food safety and the pharmaceutical industry. An initial review of analytical techniques commonly used in laboratories (ICP-MS, ICP-OES, F-AAS, GF-AAS) showed that natural freshwater often contains many analytes at concentrations below the detection limits of less sensitive methods. Therefore, the candidate material was enriched to broaden its applicability across analytical techniques.

The present work also covers metrologically critical stages of candidate CRM evaluation, including homogeneity assessment, short- and long-term stability studies, and the certification framework. Certification was further supported by external characterisation involving multiple laboratories and by an interlaboratory comparison study. Together, these steps are essential to demonstrate fitness for purpose, metrological traceability, and comparability of measurement results. The entire production process was carried out in accordance with the ISO 17034, the international standard for reference material producers.

The project “Development of a multifunctional matrix reference material: Multifunctional Polish Natural Waters (MPWN) with certified levels of metals, inorganic ions, and microplastic residues to ensure measurement traceability for Polish laboratories" is funded by the Ministry of Science and Higher Education under the Polish Metrology II Program, based on contract no. PM-II/SP/0061/2024/02 dated 15.02.2024.
The research was carried out at the Biological and Chemical Research Centre, University of Warsaw, established with co-financing from the European Union through the Operational Programme Innovative Economy 2007–2013.

(P-2)

How plasma-based analysis techniques enhance battery research

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In times of increasing energy usage, lithium ion batteries (LIBs) proved themselves a necessity in everyday life. Subsequently, great focus lies on the increase of energy density, power and safety. In state-of-the-art systems, battery cells consist of a negative electrode, which uses artificial graphite as the active material, and a positive electrode, which may use different materials depending on the application. Here, layered transition metal oxides (LiMO2; M = Ni, Mn, Co in various ratios, also known as NMC) or olivine-structured LiFePO4 stand out as the most promising materials. The stoichiometric ratio of the transition metals (TM) has a significant influence on the performance, safety and the economic impact of the battery systems.

While the production and the development of new battery cells is growing steadily, it is important to understand the degradation of the current technology. Over time, LIBs and their sodium equivalents sodium ion batteries (SIBs) suffer from fading of the capacity, leading to decreasing electrochemical performance. This is caused by several degradation processes in the system e.g. mechanical deterioration of the active material, parasitic side reactions or the migration of transition metals to the negative electrode. To better understand the extent of these phenomena, plasma-based techniques provide deep insights into the exact causes of these degradation processes.

For this, ICP-OES, ETV-ICP-OES, ICP-TOF-MS and LA-ICP-MS techniques were applied in post mortem analysis. ICP-OES and ETV-ICP-OES methods were utilized for investigations of elemental composition and distribution in the battery cell, whereas LA-ICP-MS was performed for imaging of transition metal deposition on the negative electrode after cross-electrode migration. Finally, SP-ICP-OES and SP-ICP-TOF-MS allow the analysis of the electrode active material on the particle level. Exemplary applications are the inhomogeneous state-of-charge distribution of the cathode material and the characterization of different NMC compositions within a mixed powder.

(P-3)

Fluorine depth profiling of lithium ion battery electrodes via glow discharge-sector field-mass spectrometry

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State-of-the-art lithium ion batteries are composed of composite electrodes. The electrodes contain not only electrochemically active materials to store and release energy but also conductive agent to improve electronic conductivity and a binder serving as an adhesive to obtain a mechanically stable layer of particles. On the side of the positive electrodes polyvinylidene difluoride (PVdF) is usually applied as binder. This type of polymer is only soluble in a few solvents of which N-Methyl-2-pyrrolidone (NMP) is the most common choice. During electrode manufacturing a dispersion of the materials mentioned before is produced and coated on metal foils followed by a drying process. If the drying parameters are not perfectly adjusted to the choice and composition of the materials, so-called binder migration can occur. This undesired phenomenon leads to an inhomogeneous distribution of the binder and impaired mechanical and electrochemical properties of the electrode.

To analyze the binder distribution, e.g., for quality control, cross-sectional secondary electron microscopy (SEM) combined with energy-dispersive X-ray spectroscopy (EDX) can be applied. However, this technique is very time consuming potentially leading to high amounts of production scrap, if an inhomogeneous binder distribution is found.

This poster presents a much faster way to analyze the binder distribution inside battery electrodes by applying glow discharge-sector field-mass spectrometry (GD-SF-MS). In contrast to typical inductively coupled plasmas for analytical purposes, the GD plasma enables an ionization of fluorine. Since PVdF is the only fluorine source in the samples, the F^+ ion beam ratios represent the binder depth profiles. In a first approach GD-SF-MS provided reliable binder depth profiles in no more than 15 minutes, which offers a significant advantage to battery electrode manufacturers.

(P-4)

Application of ICP-MS for multi-element analysis of iodine and trace elements in brown seaweed: a seasonal study of Fucus vesiculosus

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Inductively coupled plasma mass spectrometry (ICP-MS) is a powerful tool for multi-element analysis in complex biological matrices, enabling sensitive and simultaneous quantification across a wide concentration range. In this work, ICP-MS was applied to investigate the elemental composition of the brown seaweed Fucus vesiculosus, with particular focus on iodine as a challenging and variable analyte. comprehensive analytical approach was employed to determine iodine together with a suite of macro- and trace elements (Na, Mg, P, K, Ca, Mn, Fe, Co, Zn, V, Cr, and Se) and potentially toxic elements (Hg, Al, As, Cd, Ni, and Pb). Biomass samples collected bi-monthly over a two-year period from the Danish Baltic Sea coast provided a robust dataset for evaluating temporal variability and demonstrating the applicability of ICP-MS to long-term environmental and biological monitoring. The results highlight the capability of ICP-MS to capture pronounced seasonal variation in iodine concentrations, as well as concurrent fluctuations in multiple elements within a complex organic matrix. The study also illustrates analytical challenges associated with iodine determination and the importance of consistent methodology for reliable quantification. Multi-element data further enable integrated assessment of nutritional and potentially toxic elements within a single analytical framework.

Overall, this work demonstrates the versatility and robustness of ICP-MS for multi-element profiling in seaweed, emphasizing its value in environmental, food, and biological applications where matrix complexity and temporal variability are critical factors.

(P-5)

Assessing sodium plating and transition metal deposition on hard carbon anodes in commercial sodium ion batteries by means of plasma-based techniques

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Sodium ion batteries (SIBs) are emerging as a promising alternative to commercially established lithium ion battery (LIB) technologies. The widespread natural abundance and lower cost of sodium make the systems particularly attractive for stationary energy storage. Given that the fundamental working principles of SIBs closely resemble those of LIBs, they are considered a "drop-in" technology. Consequently, existing manufacturing infrastructure and accumulated technological know-how can be largely transferred.[1]

While on the cathode side the choice of active material remains largely the same, hard carbon (HC) has emerged as the preferred anode material in SIBs, as graphite, the state-of-the-art anode active material of LIBs, is not viable due to the limited intercalation capability of sodium ions. Nevertheless, the practical implementation of HC remains challenging, with sodium plating representing a critical issue. During charging, the potential of sodiated HC approaches the deposition potential of metallic sodium (0 V vs. Na/Na^+), whereas lithium intercalation into graphite occurs at higher potentials.[2] Under more demanding operating conditions, sodium plating is unavoidable, leading to continuous loss of cyclable sodium inventory and raising safety concerns due to higher a likelihood of short circuits.

The presented poster provides insights into the investigation of sodium plating in commercially available HC||layered oxide sodium ion batteries. Quantitative analysis of the plated sodium amount is conducted by gas chromatography coupled with a barrier ionization detector (BID), making use of the stochiometric reaction between metallic sodium and water with the sodium content determined from the amount of evolved hydrogen in the gas phase.[3] Besides that, laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) was carried out to obtain spatially resolved information on sodium plating as well as the deposition of transition metals on the hard carbon surface. The analysis was performed on cells cycled under varying temperatures, allowing a systematic assessment of the extent of sodium plating under low temperature operation.

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3. T. Brake, et al., *J. Electrochem. Soc.,* 172(8), 80540 (2025).

(P-6)

ICP-TOF-MS and HRAM-MS in the field of battery research, production and recycling – from single particle analysis to molecular imaging

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Rechargeable battery systems, especially Li-ion batteries (LIBs), play a crucial part in the transition from fossil fuels to renewable energy. The growing demand on LIBs does not only affect the production rates but also increases the need on efficient recycling strategies and waste control. Although modern LIBs already offer good performance and long lifespan (>15 years), aging phenomena still occur which lead to the end-of-life (EOL) of a battery. Understanding these aging effects is of utmost importance, not only for improving the lifespan of a battery but also for the development of recycling strategies.

One occurring aging mechanism is the loss of capacity due to the inactivation of single particles of the electrode active material. This inactivation is caused by, *e.g.*, particle cracking or loss of electronic or ionic contact between particles. Moreover, insufficient particle contact during manufacturing can also result in inactive particles in pristine electrodes. Hence, the characterization and quantification of inactive particles are inevitable to understand and determine the extent of this aging effect. With single-particle inductively coupled plasma- optical emission spectroscopy (spICP-OES) it was demonstrated, that active and inactive particles can be differentiated by the ratio between Li and the transition metals.[1-3] However, spICP-time of flight-mass spectrometry (spICP-TOF-MS) is a promising technique to gain deeper insight into the stoichiometry of the particles as well as into the distribution and heterogeneity between active and inactive particles, due to a higher sensitivity and higher scan rates of up to 12.5 kHz.

In addition to the electrodes, the electrolyte is also affected by aging mechanisms. $LiPF_6$ is most commonly used as conducting salt, however, it is also chemically as well as thermally unstable. In combination with the organic solvents and additives of the electrolyte, organophosphates and organofluorophosphates are formed during the life of a battery. The characterization of these aging products is not only important for improving the composition of the electrolyte, but to monitor the waste water during recycling processes. Liquid and/or ionic chromatography (LC/IC) hyphenated with high resolution accurate mass-mass spectrometry (HRAM-MS) allows for the identification of new aging products and their possible transformation route. By coupling HRAM with matrix assisted laser desorption ionisation (MALDI) surfaces and interphases can be analyzed with spatial resolution. For instance, the determination and localization of oligo- and polymers on the electrode surface is crucial for the development of new film-forming additives.

(P-7)

Investigating the diversity in arsenic speciation in mushrooms

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Fungi represent a highly diverse kingdom comprising millions of species [1]. Many arsenic species present in mushrooms have already been identified [2–4], with most cationic arsenic species having biologically relevant nitrogen analogues. For example, the metabolites arsenocholine and arsenobetaine exist in both arsenic and nitrogen forms.

In general, many questions remain regarding arsenic metabolism in mushrooms, particularly whether arsenic species are acquired from the soil or formed via transport and transformation pathways from structurally similar nitrogen compounds, and whether this reflects chemical substitution or a functional role in the organism. Therefore, existing knowledge on natural compounds containing the trimethylammonium group provides a basis to investigate the occurrence of trimethylarsonium-containing compounds in mushrooms.

Herein, we show the striking contrast in the arsenic speciation profiles between different types of mushrooms and highlight that studying this contrast in mushrooms may provide new insight into the biochemistry of arsenic in nature. Using optimized analytical methods based on molecular and element-selective detection, we investigate the correlation between arsenic compounds and their nitrogen analogues to shed light into the biochemical relationship between arsenic and nitrogen and the origin of natural occurrence of arsenic compounds in our environment.

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(P-8)

Is arsenic essential?

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Marine macroalgae inhabit arsenic-rich coastal environments and are routinely exposed to oxidative stress. Algae can accumulate high concentrations of arsenic, primarily as arsenosugars and arsenolipids. While the formation of these compounds has traditionally been regarded as a detoxification mechanism, their widespread natural occurrence and persistence in algal tissues suggest they may also serve important biological functions. Supporting this idea, Pétursdóttir et al. (2016) reported a linear correlation between arsenolipid concentrations and reactive oxygen species (ROS).

In this study, analytical techniques including HPLC-ICP-MS and ESI-qTOF-MS, are used to investigate whether concentrations of organoarsenicals differ in the brown seaweed *Fucus spiralis* exposed to UV-induced oxidative stress and normal light conditions. Integration with proteomic and transcriptomics will confirm if these compounds are used as cellular protection in *Fucus spiralis*. Two-way ANOVA revealed that concentrations of key arsenosugars (As-SO_3 and As-SO_4) increased significantly with elevated arsenic exposure and rose further under UV-induced oxidative stress compared with normal light conditions. In addition, samples exposed to UV-induced oxidative stress in arsenic-spiked seawater (20 µg L^{-1}) showed significantly higher concentrations of arsenophospholipids than those maintained under normal light.

Together, these findings indicate an adaptive biochemical response to combined arsenic and oxidative stress and suggest that *Fucus spiralis* may utilize arsenic-containing metabolites as a protective mechanism against oxidative damage.

Pétursdóttir, Á. H., Fletcher, K., Gunnlaugsdóttir, H., Krupp, E., Küpper, F. C., & Feldmann, J. (2016). Environmental effects on arsenosugars and arsenolipids in Ectocarpus (Phaeophyta). *Environmental Chemistry*, *13*(1), 21–33. https://doi.org/10.1071/EN14229

(P-9)

Temperature-programmed desorption / pyrolysis coupled to direct analysis in real time fourier transform ultrahigh resolution Orbitrap mass spectrometry for the analysis of natural organic matter

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Understanding the molecular composition of soil and natural organic matter (NOM) is central to quantifying carbon cycling, contaminant transport and ecosystem processes. Most current workflows rely on lengthy extractions of soils and sediments with toxic organic solvents, followed by fractionation and electrospray high resolution mass spectrometry, which are prone to ion suppression, adduct formation and a bias toward polar, extractable fractions. Ambient ionization could bypass much of this sample preparation, but has rarely been applied to highly heterogeneous NOM. Direct Analysis in Real Time (DART) offers rapid, preparation-free measurements, yet volatility and matrix effects still limit the range of detectable compounds. Here, we couple a temperature-programmed desorption/pyrolysis unit (TD-Py) to a DART source and a ultrahigh resolution tribrid Orbitrap, building an ambient TD-Py-DART-Orbitrap setup for untargeted NOM analysis. The TD-Py module applies a controlled 50–600 °C ramp, adding a volatility/thermal-stability dimension while keeping the workflow simple and fast.

We first test the system with plant-derived standards spanning major biogeochemical families (phenolics, polyphenols, terpenoids, alkaloids, curcuminoids, coumarins, glucosides, lactones) in positive and negative ion modes, and observe efficient desorption and ionization across a wide polarity and mass range, with relatively few adducts or dimers compared to ESI-based approaches. The method is then applied to several humic acids, dissolved and soil organic matter, and biochar. For humic acids, temperature-resolved total ion chromatograms separate a low-temperature domain (50–300 °C) dominated by oxygen-rich, labile compounds from a high-temperature domain (300–600 °C) enriched in refractory condensed and polyaromatic structures, consistent with thermal analysis and pyrolysis-GC/MS studies.

Ultrahigh-resolution spectra and Van Krevelen plots underline the complementarity of the two polarities: negative ion mode favors oxygenated CHO species, while positive mode emphasizes hydrocarbons and CHON/CHOS classes. Across the temperature windows, hundreds of formulas are assigned, allowing us to follow decarboxylation, dehydration, aromatization and progressive N/S incorporation into condensed aromatic frameworks, and to clearly distinguish NOM samples with different origins and degrees of humification. TD-Py-DART-Orbitrap thus offers a practical ambient ionization platform for rapid, chromatography-free, molecular-level characterization of NOM and other complex organic matrices.

(P-10)

Elemental interference uncovered: How alkali and alkaline earth metals influence $[BaF]^+$ and $[SrF]^+$ methods for fluorine analysis using ICP-MS/MS

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In response to upcoming regulatory limits on PFAS in food packaging within the European Union (effective August 2026), the demand for fast, sensitive, and reliable analytical methods for fluorine determination has increased significantly. Inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) represents a suitable analytical approach for fluorine determination due to its rapid analysis times and multi-element detection capabilities.

Direct determination of fluorine by ICP-MS/MS is not feasible because of its high first ionization energy (17 eV), which exceeds that of argon (15 eV).[1] Consequently, indirect approaches based on the formation of metal–fluoride adduct ions have been developed. The $[BaF]^+$ method is widely used, as barium exhibits a relatively high bond dissociation energy (6.39 eV for $[Ba\text{-}F]^+$: 4.00 eV for $[Ba\text{-}O]^+$) and a comparatively low second ionization potential (10 eV), both of which favor efficient adduct formation. However, $[BaF]^+$ formation appears to be significantly influenced by the presence of alkali and alkaline earth metals, leading to matrix-dependent signal variations. To address these limitations, an alternative approach based on $[SrF]^+$ formation was investigated. Its slightly lower bond dissociation energy for $[SrF]^+$ (5.43 eV; in comparison for $[SrO]^+$: 3.06 eV) and higher second ionization potential of 11 eV result in signal intensities that are approximately half of those observed for the $[BaF]^+$ method.[2] Despite this limitation, the $[SrF]^+$ approach may offer improved robustness with respect to matrix interferences.

In this study, both $[BaF]^+$ and $[SrF]^+$ methods were systematically evaluated with respect to matrix effects induced by increasing concentrations of alkali and alkaline earth elements in standard solutions. Based on the observed trends, potential mechanisms influencing metal–fluoride adduct formation in the plasma are discussed.

Overall, this work emphasizes the importance of understanding plasma-chemical processes governing adduct formation and provides a comparative assessment of the $[BaF]^+$ and $[SrF]^+$ methods as complementary strategies for fluorine determination in complex matrices.

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(2) Jamari, N. L. A.; Behrens, A.; Raab, A.; Krupp, E. M.; Feldmann, J. Plasma processes to detect fluorine with ICPMS/MS as [M–F] + : an argument for building a negative mode ICPMS/MS. *J. Anal. At. Spectrom.* **2018**, *33*, 1304–1309.

(P-11)

Determination of major and trace elements in plant-based foods by ICP-MS

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Growing consumer concerns over animal welfare, environmental sustainability, and the health benefits of plant-derived diets have driven substantial investment in the plant-based food sector. Ensuring the nutritional integrity and safety of these products requires rigorous monitoring of both essential and toxic elements across raw materials and finished goods, in compliance with regulatory standards.

This study presents a validated method for the simultaneous determination of major and trace elements in plant-based food matrices using PerkinElmer's NexION 2200 ICP-MS coupled with microwave-assisted acid digestion via the MPS 320 system. The Extended Dynamic Range (EDR) capability of the instrument enabled quantification of both major and trace elements within a single analytical run. A helium-based kinetic energy discrimination (KED) collision mode provided adequate interference removal across most analytes; however, dynamic reaction cell (DRC) mode with oxygen as the reaction gas yielded improved sensitivity and lower detection limits for arsenic and selenium.

Method performance was evaluated against EAM 4.7 criteria, with all quality control benchmarks met or exceeded across detection limits, accuracy, and analytical stability. The validated approach supports a range of practical applications, including formulation development, composite sample analysis for nutrition labeling, and surveillance of heavy metal contamination in the food supply. These findings demonstrate that the NexION 2200 ICP-MS platform is well-suited for the routine elemental analysis of plant-based food products

(P-12)

Elemental analysis of mining and soil samples by ICP-MS following aqua regia digestion

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Mining remains a cornerstone of the global economy, supplying critical materials including precious metals, metal ores, rare earth elements (REEs), lithium ores, coal, and gemstones. Across all stages of the mining lifecycle — from prospecting and profitability assessment to extraction and land reclamation — accurate elemental analysis is essential. The choice of analytical technique is governed by the required detection limits and the complexity of the sample matrix. This poster presents a workflow for the multi-element analysis of mining and soil samples using inductively coupled plasma mass spectrometry (ICP-MS) following aqua regia digestion. The study highlights the performance of the PerkinElmer NexION 2200 ICP-MS in handling the demanding analytical challenges associated with high total dissolved solids (TDS) content and highly corrosive digest matrices.

The NexION 2200's integrated suite of technologies — including the patented SMARTintro™ sample introduction system, LumiCoil load coil, 34-MHz RF plasma generator, second-generation Triple Cone Interface with OmniRing, and true-quadrupole Universal Cell — collectively deliver the robustness, sensitivity, and interference management required for reliable trace elemental quantification in complex mining matrices. Together, these capabilities make the NexION 2200 a highly effective platform for routine and research-grade analysis in the mining sector, supporting applications across ore characterization, environmental monitoring, and regulatory compliance.

(P-13)

Direct determination of trace impurities in high-purity molybdenum using the NexION 1100 ICP-MS

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High-purity molybdenum (Mo) and its compounds are integral to the synthesis of scintillation materials — including molybdates of cadmium, calcium, lead, lithium, magnesium, and zinc — which serve as ionizing radiation detectors in the search for cosmic dark matter and neutrinoless double beta decay. Verifying the purity of these materials is critical to their detector performance, necessitating highly sensitive, multi-element analytical methods with low limits of detection (LODs).

While inductively coupled plasma mass spectrometry (ICP-MS) is the established technique of choice for trace analysis in high-matrix samples, molybdenum presents significant spectral challenges. Abundant Mo-oxide species formed in the plasma (MoO^+, $MoOH^+$, Mo^{2+}) create polyatomic and doubly-charged interferences that overlap with key analyte isotopes, most notably the overlap of $^{94-100}Mo^{16}O^+$ ions with $^{110-116}Cd^+$ isotopes, complicating the accurate determination of elements such as Ti, Cd, In, Te, and Ce.

This work evaluates the NexION 1100 ICP-MS — a single-analyzer, three-quadrupole design featuring Universal Cell Technology (UCT) — as a cost-effective platform for the direct analysis of 21 trace elements in high-purity Mo. Ammonia reaction mode was employed to eliminate matrix-based interferences on Ti, Cd, In, and Te, while helium collision mode effectively removed polyatomic interferences on As and Ce. The true-quadrupole Universal Cell's precise reaction control prevented the formation of secondary interferences, ensuring analytical integrity across all target analytes.

The results demonstrate that the NexION 1100, configured with dual gas channels, delivers the sensitivity, selectivity, and robustness required for routine trace characterization of concentrated and chemically challenging Mo matrices, offering a compelling solution for quality assurance in the production of high-purity scintillation materials.

(P-14)

Ultra-trace elemental analysis of ultrapure water for semiconductor applications using the NexION 5000 multi-quadrupole ICP-MS

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The relentless drive toward smaller, faster, and more energy-efficient semiconductor devices demands ever-increasing material purity. Ultrapure water (UPW) is a critical process chemical in semiconductor manufacturing, used extensively in wafer rinsing and chemical bath preparation. Even sub-ppt levels of metallic contamination can alter the electrical properties of integrated circuit components and lead to device failure. The latest SEMI F63-0521 guidelines specify target concentrations below 1 ppt for 26 elements, with stricter sub-0.2 ppt requirements for image sensor manufacturing, placing exceptional demands on analytical instrumentation.

This study presents a method for the determination of 49 elements in UPW using PerkinElmer's NexION 5000 multi-quadrupole ICP-MS, with a focus on achieving SEMI-compliant detection limits using hydrogen and/or oxygen as alternative reaction cell gases — addressing applications where ammonia is unavailable or restricted by regional regulations. The NexION 5000 combines two full-length transmission quadrupoles (Q1 and Q3) with Universal Cell Technology (UCT, Q2), enabling MS/MS and Mass Shift operation modes for highly selective interference removal. Additional system features — including the Triple Cone Interface with OmniRing™, LumiCoil™ RF coil, Quadrupole Ion Deflector, and four independent gas channels with online gas mixing — provide the sensitivity, stability, and flexibility required for ultra-trace analysis in low-matrix samples.

Quantification was performed using the method of standard addition over a 1–20 ppt calibration range. All calibration curves yielded correlation coefficients greater than 0.999. Method detection limits (MDLs) and background equivalent concentrations (BECs) for all 26 SEMI-designated elements fell substantially below current regulatory thresholds. Notably, argon-based interferences — Ar^+ on Ca^+, ArH^+ on K^+, and ArO^+ on Fe^+ — were effectively resolved, with BECs achieved in the two-digit ppq range, demonstrating the broad interference-management capability of UCT without reliance on ammonia.

These results confirm that the NexION 5000 ICP-MS, operating with O_2 and/or H_2 reaction gases, is well-suited for routine ultra-trace elemental monitoring of UPW, offering both regulatory compliance and operational flexibility across diverse manufacturing environments.

(P-15)

Determining hexavalent chromium in air filters samples from occupational exposure using IC-ICP-MS

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Airborne hexavalent chromium (Cr(VI)) is classified as a human respiratory carcinogen and may also cause other adverse health effects [1]. Determination of Cr(VI) from airborne occupational exposure presents interrelated challenges of selectivity, sensitivity, and stability.

There is a need for reliable methods for determination of Cr(VI) in air samples from occupational settings where the integrity of chromium species is maintained. In ongoing work at STAMI we are focusing on sampling, sampling media (e.g. sampling filter and pre-treatment), storage, and determination to achieve reliable Cr(VI) quantification.

We adapted the NIOSH 7605 to an IC-ICP-MS platform to enhance species-specific selectivity and sensitivity, and to quantify Cr(III) ↔ Cr(VI) interconversion using enriched isotopes. Initial testing of 114 parallel samples of stainless-steel welding fume displayed a significant loss of Cr(VI) within the first 24 hours (avg. 15 wt%), and additional significant loss (>20 wt%) after 10 and 21 days when stored at room temperature or 4°C, respectively.

These results emphasize the need to study, control, and report oxidation/reduction conditions at every stage – sampling, storage, extraction/leaching, and analysis. Further work will aim to optimize selectivity, sensitivity, and stability through controlled laboratory studies and field settings, to ensure a reliable determination of Cr(VI) exposure.

We welcome feedback and collaboration on storage and extraction buffers, sampling media and methods, interlaboratory comparison, and experiences with welding processes or other Cr(IV)-relevant processes.

1. IARC Working Group on the Evaluation of Carcinogenic Risks to Humans. Arsenic, Metals, Fibres, and Dusts, *Chromium (VI) compounds*. 2012, International Agency for Research on Cancer: Lyon, France.

(P-16)

A statistical approach to homogeneity assessment of a multifunctional plant-based CRM for metal analysis

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Reference materials play a pivotal role in ensuring the reliability and comparability of results in chemical analysis. They are widely applied in instrument calibration, method validation, quality control procedures, and interlaboratory studies. Their suitability is fundamentally determined by confirmed homogeneity and stability, as well as by the proper establishment of the minimum sample intake, which is essential for accurate measurement uncertainty estimation.

Within the MultiBio CRM project, candidate certified reference materials based on a plant matrix were developed using strawberry leaves and fruits. The material was intentionally fortified with selected trace and toxic elements, including arsenic, cadmium, mercury, and lead. Subsequently, it underwent thorough homogenization and was subdivided into individual units.

To evaluate its fitness for purpose, a comprehensive homogeneity study was conducted. The concentrations of target metals were determined using inductively coupled plasma mass spectrometry (ICP-MS). The resulting data were subjected to rigorous statistical analysis, including outlier detection, assessment of distribution normality, and analysis of variance (ANOVA), enabling the distinction between within-unit and between-unit variability.

The obtained results confirm that the material meets the criteria for homogeneity. Furthermore, the contribution of potential inhomogeneity has been appropriately incorporated into the uncertainty budget. The developed materials demonstrate strong potential for application in method validation and in ensuring the reliability of analytical results in environmental and food analysis.

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(P-17)

Comprehensive mapping of the psoriatic skin proteome using mass spectrometry

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Proteomics is a central field within contemporary biomedical research, dedicated to the large-scale study of proteins: their expression levels, structural properties, post-translational modifications, and interactions within cells and tissues. In contrast to genomics and transcriptomics, proteomics reflects the functional state of biological systems, since proteins act as the primary executors of cellular processes. Advances in high-resolution mass spectrometry, together with sophisticated bioinformatics, now allow for the simultaneous identification and quantification of thousands of proteins in complex samples. This progress has positioned proteomics as a powerful approach for investigating disease mechanisms, identifying biomarkers, and supporting the development of precision medicine.

This methodology is particularly valuable in the study of inflammatory skin disorders such as psoriasis, a chronic condition driven by immune dysregulation and characterized by a multifaceted molecular basis. Proteomic studies have revealed that psoriatic lesions display a markedly distinct protein signature compared not only to healthy skin but also to non-lesional skin from affected individuals. These alterations include proteins linked to inflammatory processes, innate immune activation, keratinocyte differentiation, tissue remodeling, and key signaling pathways such as IL-17 and IL-36. Such findings demonstrate that proteomics not only enhances insight into the molecular mechanisms of psoriasis, but also opens avenues for discovering diagnostic, prognostic, and predictive biomarkers. In the future, these advances may facilitate more precise therapeutic decisions and the implementation of personalized treatment strategies.

Ongoing research in this field is carried out in collaboration with Military Institute of Medicine – National Research Institute in Warsaw, reinforcing its translational character and underscoring the importance of integrating basic scientific research with clinical application.

(P-18)

Single-cell ICP-MS for quantifying cisplatin uptake in veterinary-relevant cell models: Bridging application and instrumentation

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Platinum-based chemotherapeutics, such as cisplatin, remain widely used in both human and veterinary oncology, yet their effectiveness is limited by toxicity and pronounced heterogeneity in cellular uptake. Conventional analytical approaches provide only bulk-average concentrations, masking cell-to-cell variability. In contrast, single-cell inductively coupled plasma mass spectrometry (SC-ICP-MS) enables direct quantification of metal content at the level of individual cells, offering new insights into drug uptake and cytotoxic effects.

In this study, SC-ICP-MS was applied to investigate cisplatin uptake in three veterinary-relevant cell lines: C26 (murine colorectal carcinoma), 4T1 (murine mammary carcinoma), and MDCK (canine kidney epithelial cells). Cells were exposed to 10–40 μM cisplatin for 24 hours, then washed and resuspended in PBS. Measurements were performed using a PerkinElmer NexION 2000 ICP-MS, equipped with a dedicated single-cell sample introduction system, comprising a CytoNeb nebulizer and an Asperon™ spray chamber, both specifically designed for the efficient and reproducible introduction of intact cells into the plasma while minimizing signal dispersion. This configuration ensures high transport efficiency and stable generation of transient ion signals from individual cells. Data acquisition and evaluation were carried out using Syngistix™ Single Cell Application Software, which provides automated detection and processing of time-resolved events, enabling reliable quantification of intracellular platinum at the femtogram-per-cell level. Together, this integrated hardware–software platform supports high-throughput and robust single-cell analysis, even in complex biological matrices.
The results showed a clear dose-dependent increase in intracellular platinum across all cell lines, with notable differences between models. In particular, 4T1 cells exhibited consistently lower platinum uptake compared to C26 and MDCK cells. Importantly, SC-ICP-MS revealed broad, often lognormal-like distributions of intracellular platinum mass, highlighting substantial heterogeneity within cell populations that cannot be captured by bulk methods. At higher exposure levels, increased particle counts indicated significant cell fragmentation, reflecting cytotoxic effects of cisplatin. These observations were supported by complementary cell counting and microscopy.

Overall, this work demonstrates that SC-ICP-MS is a powerful tool for studying metallodrug uptake and toxicity at the single-cell level in veterinary-relevant systems. The combination of high sensitivity, single-cell resolution, and compatibility with established ICP-MS workflows makes it a valuable approach for both fundamental research and applied analytical applications involving metal-based therapeutics.

(P-19)

Calibration of single-particle ICP-MS and its application on antibacterial products

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Single-particle inductively coupled plasma-mass spectrometry (sp-ICP-MS) is a powerful technique for determination of elemental content in nanoparticles and their number concentration, with minimal sample preparation. Unlike bulk solution analysis, single-particle measurement requires special attention, particularly in calibration. Nanoparticle calibration of nanoparticles is challenging due to the limited availability of reference materials and the inherent instability of nanoparticles, which tend to dissolve or aggregate. Calibration of particle number concentration and size relies on determining transport efficiency, which can be achieved through the particle frequency method, particle size method, or dynamic mass flow method. In this work, particle size calibration was explored using three approaches: ionic solutions of the same element, reference particles of the same element, and reference particles of different elements. Gold and silver nanoparticles were used as study materials.

Results showed that when reference particles of a different element were used, accuracy depended on the sensitivity ratio of the ionic standards and the intensity ratio of the particles. Thus, it was essential that the sensitivity ratio of the ionic standards matched that of the nanoparticles. Signal responses of gold and silver ionic standard solution in different solvent matrices highlighted the importance of matrix-matched calibration for nanoparticle sizing. To preserve particle number concentration and size, cloud point extraction was employed as a sample preparation method for silver nanoparticles. The mean recovery of particle number concentration exceeded 90%, and both particle size and number concentration remained stable after two weeks of storage at 4 °C. Cloud point extraction was successfully applied to extract silver nanoparticles from antibacterial products[1].

1. CHAO Jingbo, Lee Wan Waan, CHEN Zhiwei, et al. Cloud Point Extraction-Single Particle Inductively Coupled Plasma Mass Spectrometry for the Inspection and Identification of Silver Nanoparticle Antibacterial Products[J]. Chinese Journal of Inorganic Analytical Chemistry, 2026, 16(3): 488-498.

(P-20)

Three-dimensional and immuno-mass spectrometry imaging of HfO_2 nanoparticles in breast cancer tissue by LA-ICP-TOFMS

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Nanoparticle-based radiosensitizers hold great promise for enhancing the efficacy of radiotherapy. However, the complex tumor microenvironment poses significant challenges to their efficient delivery and overall therapeutic performance. In this study, we have developed a high-resolution multimodal imaging workflow that integrates three-dimensional (3D) elemental imaging based on serial sectioning and laser ablation-inductively coupled plasma-time-of-flight mass spectrometry (LA-ICP-TOFMS) with multi-elemental analysis and metal-isotope-tagged immunolabeling to investigate the spatial distribution and cellular associations of hafnium oxide nanoparticles (HfO_2 NPs) in a murine breast cancer model.
Multi-elemental imaging revealed pronounced intratumoral heterogeneity, with calcium (Ca) predominantly localized in necrotic regions, while other endogenous elements exhibited distinct spatial patterns. Notably, Hf signals from HfO_2 NPs showed limited penetration into Ca-rich necrotic cores, indicating a strong dependence of their distribution on local tissue pathology. Three-dimensional reconstruction further demonstrated that HfO_2 NPs were broadly distributed within viable tumor regions. To further elucidate nanoparticle-cell interactions, metal-isotope-tagged immunomarkers were combined with elemental imaging, enabling correlation analysis between HfO_2 NPs and cellular phenotypes at 1 μm spatial resolution. The results suggest that HfO_2 NPs enter multiple cell types within the tumor microenvironment, including epithelial cells, stromal fibroblasts, and endothelial structures. Overall, this multimodal imaging workflow reveals the complex interplay between elemental heterogeneity, tissue pathology, and nanoparticle distribution, highlighting the limitations of bulk analysis. This approach provides a powerful tool for evaluating and optimizing nanoparticle-based radiotherapeutics.

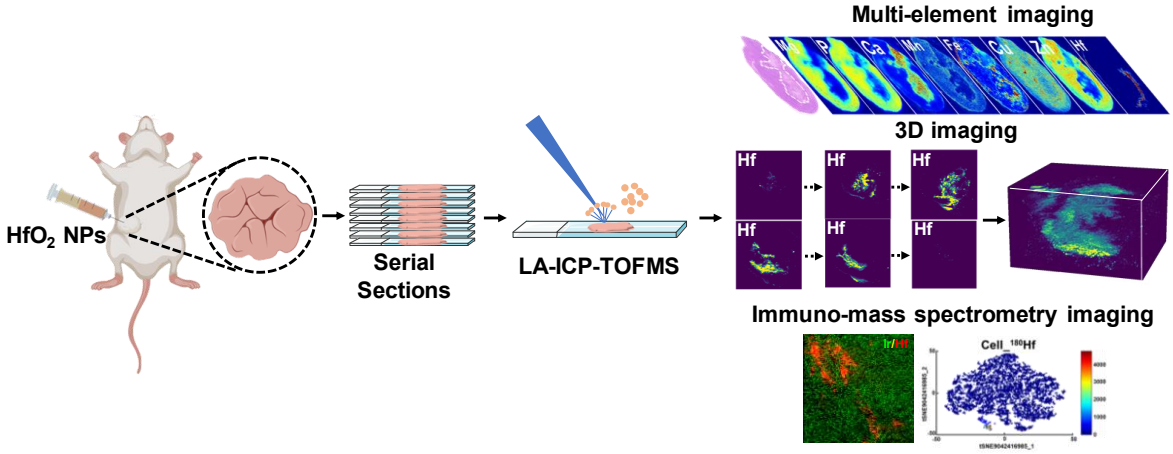

Figure 1. Schematic of the high-resolution multimodal imaging workflow integrating three-dimensional (3D) elemental imaging via serial sectioning and LA-ICP-TOFMS with metal-isotope-tagged immunolabeling for spatial and cellular mapping of HfO_2 nanoparticles in a murine breast cancer model.

(P-21)

Plasma-based CE-ICP-MS/MS study of formation and physiological alterations in cisplatin–gold nanoparticle delivery systems

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One of the main limitations of contemporary chemotherapy is the low selectivity of anticancer drugs, such as cisplatin (CDDP), causing several side effects. Consequently, Drug Delivery Systems (DDS) based on nanocarriers are being developed to improve the pharmacokinetic properties of cytostatic drugs and enable their controlled release. Gold nanoparticles (GNPs) occupy a special place among them due to their biocompatibility and rich surface chemistry.

In this study, capillary electrophoresis coupled to inductively coupled plasma ionisation tandem mass spectrometry (CE-ICP-MS/MS) was utilised to monitor the formation of GNPs-CDDP complexes and their transformation in conditions simulating the physiological environment. The effect of functional groups modifying the surface of the gold nanoparticles on the drug-binding efficiency and stability of the resulting complexes was also analysed. Particular attention was paid to the analytical capabilities offered by using a triple quadrupole mass spectrometer. The ICP-MS/MS configuration effectively eliminates spectral interference and enables selective elemental analysis using reaction gases.

The technique employed enabled the simultaneous detection of gold and platinum isotopes, allowing interactions between the carrier and the drug to be monitored directly in real time. Importantly, for the first time, a triple quadrupole mass spectrometer was used to perform quantitative analysis of sulphur in these systems, opening up new possibilities for their chemical characterisation. The high CE resolution and low limits of detection ICP-MS/MS facilitated comprehensive tracking of changes throughout the reaction mixture, providing a more complete picture of the formation mechanisms and stability of the systems under study.

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(P-22)

Characterization of gold nanoparticle–cisplatin DDSs using two different CE–ICP-MS interfaces

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Despite various advancements in anticancer therapies, to this day, one of the more frequently used drugs in the treatment of solid tumors is cisplatin (*cis*-diamminedichloridoplatinum(II), CDDP). Due to the mechanism of action, CDDP is a nonselective drug and it accumulates in cancerous as well as healthy tissues, which drastically increases the number and severity of adverse effects in patients who undergo this treatment [1]. To combat the adverse effects of using CDDP, drug delivery systems (DDS) can be used. Such systems can increase tumor accumulations, bloodstream circulation time, and cellular uptake and can provide targeted transport, and controlled release of therapeutics [2]. In this study, gold nanoparticles (GNPs) are chosen as a drug delivery system due to their nontoxicity and the possibility of covalent bonding with different chemical moieties. Furthermore, it was shown that applying GNPs as carriers for platinum-based anticancer drugs increases conjugate cytotoxicity and penetration to cancer cells [3].

Interactions between cisplatin and gold nanoparticles were studied using an inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) detector hyphenated with capillary electrophoresis (CE). ICP-MS/MS allows for simultaneous gold, platinum and sulfur (protein marker) detection during one analysis. However, the crucial part is utilizing the CE system, which allows for analyzing GNPs–CDDP DDSs by separating and identifying different forms of created complexes or partial complexes in one run.

The key technical variable in this study was interface between mass spectrometer and capillary electrophoresis system. For this hyphenation MiraMist CE nebulizer was used with two different spray chambers. In the first case nebulizer was placed horizontally and was connected to the mini spray chamber and in the second scenario vertical nebulizer was joint with Scott double-pass spray chamber. Impact of these two interfaces on GNPs–CDDP drug delivery system signal intensities, separation efficiency and analysis stability was evaluated.

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(P-23)

Evaluating the bioaccessibility of trace metals in a plant based alternative protein source, canola meal, using online leaching method coupled to inductively coupled plasma mass spectrometry

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Sustainable plant-based proteins are gaining attention as alternatives to conventional animal-based protein sources, driven by growing environmental and food security concerns. However, the presence and bioaccessibility of trace elements in alternative plant-based protein sources remain insufficiently characterized. In this study, we investigated the bioaccessible fractions of trace elements including Ti, V, Cr, Co, Ni, Cu, Zn, Sr, Mo, Cd, Ba, and Pb in a certified novel plant-based protein source, canola meal.

A continuous online leaching method coupled with inductively coupled plasma mass spectrometry was used to simulate human digestion. Solid samples were held in a filter holder unit, and simulated saliva, gastric, and intestinal fluids were sequentially passed through to mimic the physiological digestion process. Internal standards were added into the simulated fluids to correct for column-related variability, improving median standard deviations by two-fold with significant improvement for Co, Cu, Cd, and Ba, median limit of detections by seven-fold, and recoveries for Co, Ni, Cu, Zn, Sr, Cd, Ba, Pb. The performance of the method and its bioaccessibility results were compared with those obtained using a batch method. Release dynamics were investigated through cumulative signal profiles and isotopic ratio analysis. Additionally, scenario-based exposure assessments were carried out across different sex and age groups.

This study shows the potential of the online leaching method for assessing trace element bioaccessibility in food matrices, providing complementary bioaccessibility information to conventional total concentration measurements, offering a more realistic and comprehensive basis for food safety and nutritional assessments.

(P-24)

Agilent 9500 ICP-QQQ with m-lens for ultra-trace analysis of high-purity reagents

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Ultra-trace impurity analysis is increasingly required for high-purity reagents used in semiconductor processing and other advanced materials applications, where chemicals such as nitric and sulfuric acids must meet stringent contamination specifications. Analytical methods for these reagents must achieve sub-ppt level detection limits (DLs) while maintaining low instrumental backgrounds under hot-plasma conditions.

This study describes a triple quadrupole Inductively Coupled Plasma Mass Spectrometry (ICP-QQQ) workflow for the ultra-trace analysis of high-purity reagents using preset analytical methods optimized for low-matrix samples. Interference control was achieved through a combination of helium mode and reaction mode, enabling effective suppression of plasma- and matrix-derived polyatomic interferences. In parallel, low background equivalent concentrations (BECs) for easily ionized elements were achieved with optimized ion optics, supporting low-level measurements under hot-plasma conditions. Helium mode provided efficient on-mass interference removal for a broad range of trace metals, while reaction mode was applied selectively for more challenging spectral overlaps.

The method was evaluated using diluted high-purity nitric acid and sulfuric acid matrices with external, matrix-matched calibration. Excellent linearity was achieved across the calibration ranges, and sub-ppt detection limits with low BECs were obtained for most target elements in both matrices.

These results demonstrate that the combination of helium mode and reaction mode with an optimized ion-optics configuration enables sensitive ultra-trace impurity measurements of high-purity reagents. The described workflow provides a practical entry point for ultra-trace analysis of low-matrix, high-purity reagents using an ICP-QQQ system.

(P-25)

Analysis of high purity titanium using an Agilent 9500 ICP-QQQ

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Accurate determination of trace metallic impurities in high-purity titanium is essential for advanced materials applications, including semiconductor and aerospace manufacturing, where impurity levels directly influence performance and reliability. In this study, triple quadrupole Inductively Coupled Plasma Mass Spectrometry (ICP-QQQ) system equipped with a collision/reaction cell (CRC) was evaluated for the analysis of impurity elements in a high-titanium matrix.

A 200 ppm titanium solution prepared from high-purity titanium powder was analyzed using a combination of reaction modes to suppress spectral interferences arising from titanium-based doubly charged ions, oxides, and hydride species. Reaction mode employing a mixture of reactive gases enabled effective removal of interferences affecting key analytes such as Na, V, Cu, and Zn. Quantification was performed using the method of standard addition, achieving background equivalent concentrations at the low ppt level for most elements. Spike recovery experiments (n = 10) demonstrated recoveries within ±10% with relative standard deviations typically below 3%. During continuous measurements exceeding 3 hours, internal standards showed recoveries in the range of 90–120%. These results demonstrate that an ICP-QQQ under optimized reaction conditions provides robust, accurate, and reproducible ultra-trace impurity analysis in high-purity titanium matrices, supporting stringent quality-control requirements for high-technology materials.

(P-26)

Automation in trace metals analysis of engine coolants

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Preventative maintenance of heavy-duty engines relies on rapid and reliable assessment of coolant composition, particularly trace metals and additive elements that indicate wear, corrosion, and system health. This study evaluates the application of the Agilent Advanced Dilution System 2 (ADS 2) for automated sample preparation in the inductively coupled plasma–optical emission spectroscopy (ICP-OES) analysis of glycol-based engine coolants. Ten elements (Al, B, Ca, Cu, Fe, Mg, Mo, Na, P, and Si) were quantified using an Agilent 5900 ICP-OES instrument, with calibration standards and sample dilutions prepared automatically via ADS 2.

The automated workflow enabled both prescriptive and reactive dilutions, ensuring samples remained within calibration range while minimizing manual intervention. Analytical performance demonstrated excellent linearity ($R^2 > 0.99997$), robust internal standard stability, and successful quality control throughout the analysis. Precision of automated dilutions was consistently below 5% RSD and showed strong agreement with manually prepared samples (≤20% relative percent difference across all analytes).

The implementation of ADS 2 significantly reduced sample preparation time, requiring only ~20 seconds additional time per sample during analysis, while also lowering consumable usage and operator workload. These results confirm that automated dilution provides accurate, precise, and efficient coolant analysis, supporting high-throughput laboratories and improving operational efficiency in predictive maintenance workflows.

(P-27)

Enhancing lithium-ion battery production - Automated and sustainable elemental analysis using an ICP-OES

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The growing demand for high-quality lithium-ion batteries (LIBs) has intensified the need for accurate and efficient elemental analysis of battery precursor materials, including recycled and high-purity lithium salts. In this study, an Agilent 5800 Vertical Dual View (VDV) ICP-OES coupled with an ADS 2 autodilutor was employed to enable automated, high-throughput analysis of lithium carbonate and manganese sulfate samples. Semi-quantitative screening using IntelliQuant facilitated rapid identification of elemental composition and potential spectral interferences, while advanced features such as MultiCal and Fast Automated Curve-fitting Technique (FACT) ensured accurate quantification across a wide dynamic range.

Automated dilution significantly reduced manual sample preparation, improving reproducibility and minimizing contamination risks. Method performance was validated through spike recovery (92.5–107.5%), low method detection limits, and long-term stability with <3% RSD over 10 hours. The system demonstrated excellent precision and accuracy for trace and major elements in complex, high-matrix samples.

These results highlight the advantages of integrating intelligent automation with ICP-OES for LIB material analysis, supporting sustainable battery production through improved productivity, reduced waste, and enhanced data quality.

(P-28)

Microdroplets in quantitative LA-ICP-QMS: Application in depth resolved ion doping determination of semiconductors

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Laser ablation – inductively coupled plasma – mass spectrometry is a versatile analytical technique that enables spatially resolved analysis of major, minor, and trace elements in solids. However, accurate quantification is challenged by matrix effects during ablation, aerosol transport, and ionization that affect signal response. Limited availability of certified reference materials further constrains accurate quantitative analysis, often resulting in the use of non-matrix-matched standards or prompting the use of in-house matrix-matched standards that require careful optimization and validation.[1]

Other approaches combine liquid standards and LA aerosols, e.g., calibrating with pneumatic nebulization of liquid standards alongside the sample's LA aerosol.[2] In 2025, a concept introducing microdroplets of liquid standards was first combined with laser ablation for quantitative bulk multielement analysis using LA-ICP-TOFMS.[3]

Here, we adapt the droplet-based calibration strategy for LA-ICP-MS with quadrupole ICP-MS (QMS), focusing on its application in spatially resolved analysis of solids. Particular emphasis is placed on high-resolution depth profiling to evaluate the capability of this approach for accurate depth-resolved quantification. This is demonstrated using an ion-implanted silicon carbide semiconductor, and the results are systematically compared with those obtained from a non–matrix-matched calibration strategy based on a certified reference material.

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Investigation of *in vivo* Hg detoxification mechanisms by Se through elemental and isotopic analysis

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Mercury (Hg) is a toxic heavy metal, emitted into the environment as a result of natural processes and anthropogenic human activities. Once released into the atmosphere, Hg undergoes several transformations throughout its complex biogeochemical cycle and finally reaches the ocean. There, it bioaccumulates and biomagnifies in marine biota along the trophic food chain, mainly in one of its toxic forms: Methylmercury (MeHg). As a result, top predatory fish and other seafood species can contain elevated concentrations of MeHg, making the consumption of fish and seafood the primary source of human exposure to MeHg. [1]

Recent studies have shown that Selenium (Se) plays a key role as natural Hg antagonist through the formation of inert Hg-Se nanoparticles. While these interactions have been thoroughly investigated in seabirds and marine mammals, [2-4] uncertainties still remain regarding the role of specific organs in the detoxification process and the internal dynamics of both Hg and, especially, Se in marine fish. [2,5] Our preliminarily study on the determination of the Se isotopic signature in several organs of a Bluefin Tuna fish revealed similar trends between Se and Hg isotopic signatures in the organs analyzed, particularly in the spleen and the kidney. [6] These initial results suggest that combined Se and Hg isotopic analysis may show potential as a powerful approach to further investigate their metabolic pathways in marine fish and to further elucidate the role of Se in Hg detoxification.

Building on these preliminary findings, we are now aiming at a better understanding of Se and Hg interactions in marine fish by exploring another marine species, Atlantic Halibut. In this context, Hg and Se elemental contents, Hg speciation, and Hg isotopic signatures were determined across several organs, including liver, kidney, muscle, spleen, intestine and brain. Prior to the characterization of Se isotope ratios in these aforementioned samples, the sample preparation procedure, including the chromatographic isolation of Se using Thiol Cellulose powder (TCP), previously reported in the literature [6], was revisited and further improved. By integrating isotope ratio data with elemental speciation, this work eventually aims to contribute to the unraveling of the internal dynamics of Hg and Se in marine organisms and the understanding of the role of Se and specific organs in the detoxification process of Hg.

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