

**BNASS 2024: The 21st Biennial National Atomic Spectroscopy Symposium**

**11th – 13th September 2024, Burlington House,  
The Royal Society of Chemistry, London**



**RSC INTEREST GROUP  
ATOMIC SPECTROSCOPY**

**BNASS is the flagship meeting for the Atomic Spectroscopy Group  
of the Analytical Community, Royal Society of Chemistry**



## Preface

On behalf of the Organising Committee for the 21<sup>st</sup> Biennial National Atomic Spectroscopy Symposium (BNASS) and the Atomic Spectroscopy Group (ASG), we would like to welcome you all and thank you for your contributions and participation! A lot has happened since BNASS 2022 but we are very much looking forward to catching up.

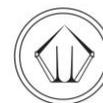
The philosophy of BNASS is to encourage the exchange of ideas and knowledge within analytical atomic spectroscopy field with a mix of established and early career speakers. BNASS is celebrating its 21<sup>st</sup> event and during its history, there have been some tremendous changes in atomic spectroscopy. These advances have been showcased at BNASS, which has built an international reputation for both the quality of the science presented and the unique style of the symposium, enabling delegates to meet and discuss issues in a social setting.

This year, we are returning to the 3 day format and find ourselves in the home of the Royal Society of Chemistry at Burlington House in London. It's roots began in the 1660s, with the Earl of Burlington taking over in 1704, lending his name to the building. Over the years, it has had a multitude of alterations and uses. Currently, Burlington House also hosts the:

- [Geological Society of London](#)
- [Royal Academy of Arts](#)
- [Royal Astronomical Society](#)
- [Society of Antiquaries of London](#)
- [Linnean Society of London](#)



Please enjoy BNASS 2024 and hope that you take full advantage of the networking opportunities with the speakers, attendees and exhibitors. As chair, I would like to thank the organising committee and ASG for their support and dedication.



## Organising Committee

**ASG Chair:** Dr Sarah Hill, National Measurement Laboratory, LGC

**Treasurer:** Dr Jackie Morton, Biological Monitoring, Health & Safety Executive

**Programme Coordinator:** Dr Shaun Lancaster, University of Leoben

**Social Coordinator:** Dr Rebekah Moore, Imperial College London

**ASG Secretary:** Dr Andy Fisher, Plymouth

**ASG Committee:** Dr Adam Laycock (UK Health Security Agency), Prof Steve Hill (University of Plymouth), Dr Elliot Hamilton (British Geological Survey).

## Social Events

On both evenings, we will be hosting events to enable the opportunity to continue discussions from the day and catch up. On Wednesday, we have reserved the Paradiso Burger & Cocktail Bar, overlooking the Southbank along the Thames, which will feature a quiz! On Thursday, just a stone's throw from Piccadilly Circus, Neon 194 will also feature a live band!



## Wednesday Evening

### Paradiso Burger & Cocktail Bar

Gabriel's Wharf,  
Southbank,  
SE1 9PP  
Balcony overlooking the river  
From 7.30pm  
<https://paradisoburger.com/>



## Thursday Evening

### Neon 194

194 Piccadilly  
W1J 9LN  
From 7pm  
Including a live band!  
<https://www.neon194.com/>



[Link to Google Maps Route with Walking Directions](#)



## The Phil Riby Award

Phil was an active member of the Atomic Spectroscopy Group and a big component of BNASS, being the conference chair of the 18th meeting in Liverpool, on the organising committee of 19th in London, and was instrumental in bringing BNASS to Manchester in 2022. His enthusiasm, drive and cheerful nature is still greatly missed. Phil was a people person and a champion for younger scientists, the welfare and success of his students was always his priority. To commemorate Phil's contribution to BNASS, education and the wider atomic spectroscopy community, the Phil Riby prize was announced at BNASS 2022 for the best student presentation at the conference. He was a passionate supporter of early career scientists and the prize provides an opportunity to present a lecture at the next BNASS.

## Roundtable Discussions

This year we are introducing two roundtable discussions to gather your thoughts and opinions on important and relevant topics: Sustainability in the Laboratory and Equity, Diversity and Inclusion in Science. Both sessions are being facilitated by the RSC.

### **Making our science greener session at BNASS**

Science and technology are key to a more sustainable future – from clean energy technologies to tackling disease – and laboratories are essential to carrying out the research, analysis and teaching that underpin these advances. However, laboratory buildings, processes and equipment, by their nature, can be resource and energy intensive. During this session, facilitated by the BNASS Committee you will hear a short presentation from Anne Horan on some key findings from the RSC's Sustainable Labs report based on a survey of 700 practising scientists, combined with desk research and insights from expert working groups, in our [Sustainable Labs](#) report and [Resource Hub](#). There will be opportunity for attendees to share and discuss their ideas for ways to drive forward lab sustainability in the chemical sciences.

### **Equity, Inclusion & Diversity session at BNASS**

It is generally recognised that to get the very best scientific outputs we need a diversity of inputs and talents. However, progress is still slow and yet not well understood or actioned on how to truly achieve diversity and how to ensure that those diverse inputs and talents are included, accepted, valued and empowered. Current evidence shows that there is a continuous struggle for equality in science, particularly in attracting, retaining and developing talented people from underrepresented groups into positions of leadership. During this session, facilitated by the BNASS Committee you will hear a short presentation from the Royal Society of Chemistry I&D



team on recent evidence and interventions to make the chemical sciences fairer and more inclusive for everyone. The presentation hopes to stimulate discussions across attendees on a broad range of topics including creating an inclusive research culture and challenging the traditional measures of success.

- [1] [Diversity landscape of the chemical sciences](#)
- [2] [Breaking the barriers: Women's retention and progression in the chemical sciences](#)
- [3] [Exploring the workplace for LGBT+ physical scientists](#)
- [4] [A sense of belonging in the chemical sciences](#)
- [5] [Missing elements: Racial and ethnic inequalities in the chemical sciences](#)
- [6] [Is publishing in the chemical sciences gender biased?](#)

## Acknowledgements

The Organising Committee wishes to express its grateful thanks to the following organisations for their generous support. BNASS 2024 would not be possible without their involvement and we strongly encourage all attendees to take some time out of the schedule and visit the Vendors Exhibition.

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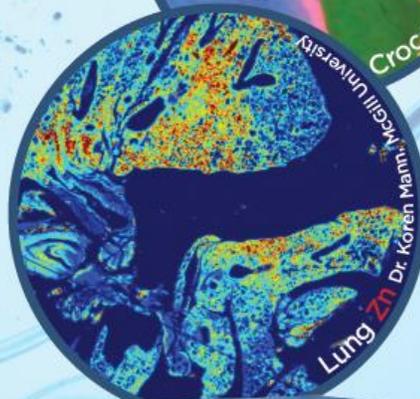
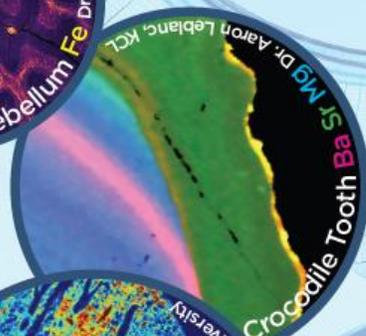
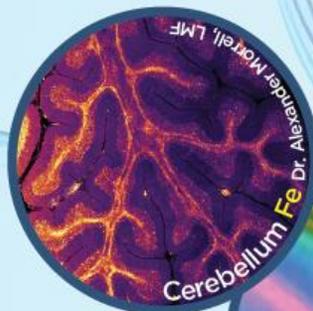
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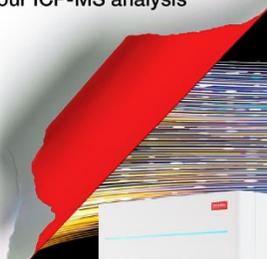
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1 NOTE: Revenue amounts are based on TTM through Q2 2024 before intercompany eliminations

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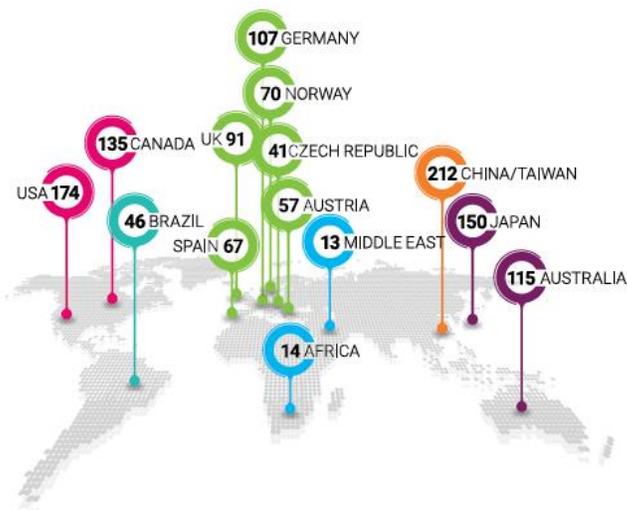
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The Royal Society of Chemistry publishes over 50 world-leading journals that span the core chemical sciences and related fields. Known for rigorous, fair peer review and fast publication times, our journals publish the best science, from original research articles to authoritative reviews.



## Programme

Time	Wednesday 11 <sup>th</sup> September: Main Programme
12:30-13:30	Registration and Lunch
13:30-13:40	<b>Welcome address:</b> BNASS 2024 Organising Committee
<b>Session 1: Laser Ablation and Instrumental Advances</b>	
13:40-14:20	<u>Keynote:</u> Thibaut van Acker, Ghent University, Belgium The occurrence and drawbacks of two-phase aerosol transport upon ablation of soft biological matrices using nanosecond laser ablation-inductively coupled plasma-mass spectrometry
14:20-14:40	Nathan Westwood, Loughborough University, United Kingdom The application of LA-ICP-MC-MS for quantified, high spatial resolution imaging of Pb-Pb isotope ratios in ferromanganese crusts
14:40-15:00	Amy Lovejoy, Imperial College London, United Kingdom The effect of histological processing on indigenous elemental content and distribution in breast tumour tissue sections
15:00-15:30	Refreshment break
15:30-15:50	Phil Shaw, Nu Instruments, Wrexham, United Kingdom “Please sir, can I have some more?” – more elements, more dynamic range, more pixels, more samples! Getting the most out of time of flight ICP-MS and kHz laser ablation systems.
15:50-16:10	David Price, PerkinElmer, Seer Green, United Kingdom Overcoming High-Complexity ICP-MS Tasks
16:10-16:30	Raimund Wahlen, Agilent Technologies, Stockport, United Kingdom Aerosol or liquid? A comparison of different dilution strategies for high-matrix ICP applications, including new automation approaches to reduce manual tasks in the lab.
16:30-17:00	Flash poster presentations
17:00-18:00	Poster session with refreshments
19:30	Evening Social Event – Paradiso on the South Bank



Time	Thursday 12 <sup>th</sup> September: Main Programme
<b>Session 2: Spectroscopy in Aquatic Systems</b>	
09:30-10:10	<u>Keynote:</u> Susan Little, University College London, United Kingdom Metal stable isotopes in the marine realm
10:10-10:30	Hui Xu, Imperial College London, United Kingdom Isotopic constraints on the biological and atmospheric controls of cadmium distribution in the Tropical North Atlantic
10:30-10:50	Bankole Walter Osungbemi, University of Strathclyde, Glasgow, United Kingdom Effect of different weathering processes on the adsorption of arsenic, cadmium, chromium and lead on polyethylene, poly(ethylene terephthalate), polypropylene and poly(vinyl chloride) microplastics
10:50-11:20	Refreshment break
11:20-11:40	David King, British Geological Survey, Nottingham, United Kingdom and Nottingham Trent University, United Kingdom A novel, robust field-sampling method for preserving mercury species associated with waters related to artisanal gold mining
11:40-12:00	Abayneh Ataro Ambushe, University of Johannesburg, South Africa Speciation of mercury in sediments using high performance liquid chromatography hyphenated to inductively coupled plasma-mass spectrometry and a thermo-desorption technique
12:00-12:20	Shaun Lancaster, Montanuniversität Leoben, Austria An unconventional approach to the determination of oxygen isotope ratios in water using inductively coupled plasma – tandem mass spectrometry
12:20-13:20	Lunch and poster session
13:20-14:10	<b>Roundtable Discussion – Sustainability in the Laboratory</b>
<b>Session 3: Single Particle and Single Cell ICP-MS</b>	
14:10-14:50	<u>Keynote:</u> David Clases, Universität Graz, Austria Gaining new perspective on the nano- and microscale: Combining elemental mass spectrometry and optical methods to characterise single particles
14:50-15:10	Elizabeth Leese, HSE, Buxton, United Kingdom Biomonitoring for respirable crystalline silica: the determination of Si-containing particles in exhaled breath condensate using single particle inductively coupled mass spectrometry.
15:10-15:30	Refreshment break
15:30-15:50	Ariane Donard, Nu Instruments, Wrexham, United Kingdom When is a particle of interest? Single particle time of flight ICP-MS as a tool to determine particle numbers and true compositions.
15:50-16:10	Antonio Bazo, University of Zaragoza, Spain Revisiting single-particle ICP-mass spectrometry (SP-ICP-MS) approaches for micro/nano quantification of discrete entities



16:10-16:30	Rob Clough, University of Plymouth, United Kingdom A fish tissue reference material certified for Ag nanoparticles? Progress so far.
16:30-16:50	Philip Holdship, University of Oxford, United Kingdom Precise quantification of metal uptake in cells by single cell ICP-MS
16:50-17:10	Refreshment break
17:10-18:00	<b>Roundtable Discussion – Equity, Diversity and Inclusion in Science</b>
19:00	Evening Social Event - Conference Dinner at Neon 194

Time	Friday 13 <sup>th</sup> September: Main Programme
<b>Session 4: Environmental Analysis</b>	
09:30-10:10	<u>Keynote</u> : Tea Zuliani, Jožef Stefan Institute, Slovenia High-precision analysis of non-traditional isotopes in environmental research
10:10-10:30	Emma Braysher, National Physical Laboratory, Teddington, United Kingdom Isotope ratio measurements using ICP-MS/MS for source attribution of priority pollutants in air
10:30-10:50	Pierre Couture, Surrey Ion Beam Centre, Guildford, United Kingdom Passive air quality investigation of leaves, moss and trees using Ion Beam Analysis techniques
10.50-11.30	Refreshment break
11.30-11.50	Julian Cardini, Technical University of Denmark, Kongens Lyngby, Denmark Advancements in Multi-Element Speciation: A Novel Approach for the Identification of Chelating Compounds Using SEC-ICP-MS/MS and SEC-QTOF-MS with a Focus on Cadmium in Plant-Based Foods
11.50-12.10	Hau Lam Jody Cheong, National Physical Laboratory, Teddington, United Kingdom Characterising chemical composition in brake wear using tandem inductively coupled plasma mass spectrometry (ICP-MS/MS)
12.10-12.30	Saskia Burke, National Physical Laboratory, Teddington, United Kingdom Measurement of cosmogenic Silicon-32 using inductively coupled plasma tandem mass spectrometry
12.30-12.50	Emma Braysher on behalf of Ben Russell, National Physical Laboratory, Teddington, United Kingdom Investigating inductively coupled plasma tandem mass spectrometry for measuring challenging radionuclides in steel samples as part of an interlaboratory comparison exercise
12:50-13.00	<b>Close and Final Remarks: BNASS Organising Committee</b>
13:00	Lunch and depart



## Keynote Speakers



**Dr. ir. Thibaut Van Acker** is a postdoctoral researcher in the Atomic & Mass Spectrometry research unit of Ghent University, which is led by Prof. Dr. Frank Vanhaecke. He is an expert in fundamentals, analytical method development and applications of LA-ICP-MS in multi-disciplinary contexts. He is co-author of over 30 scientific publications in peer-reviewed international journals and contributed to over 60 conference presentations on major international conferences. Recently, he also won the European Rising Star Award for Plasma Spectrochemistry 2023 at the European Winter Conference on Plasma Spectrochemistry.

<https://orcid.org/0000-0002-0649-7228>

**Dr Susan Little** graduated with an MSci Natural Sciences degree from the University of Cambridge in 2009, and then went on to complete a PhD in Isotope Geochemistry at the University of Bristol. She then undertook postdoctoral research at ETH Zurich between 2013 and 2015, before becoming a Postdoctoral Research Fellow at Imperial College London. In 2019, Dr Little became a lecturer at the department of Earth Sciences, University College London, and then Associate Professor in Isotope Geochemistry in 2023. She was co-chair of the Diversity, Equity and Inclusion committee for the European Association of Geochemistry between 2021-



2024. Dr Little's research focuses on developing novel tracers of carbon cycling in the past and present oceans. Her recent work on Greenland fjords highlights the potential of metal isotopes (Ni, Cu and Zn) as tracers of past Earth system climate perturbations.

<https://orcid.org/0000-0002-9957-2636>



**Prof. Dr. David Clases** graduated with a Master in Chemistry at the University of Münster, Germany in 2014. He then went on to complete a PhD on trace metals in medicine and the environment. Between 2017 and 2021, he held postdoctoral fellow and lecturer positions at the University of Technology in Sydney, Australia, before going on to become an Assistant Professor for Analytical Chemistry at the Institute of Chemistry, University of Graz, Austria.



His most recent work focuses on the multimodal characterisation of nano- and microstructures at environmental levels. He has just been awarded an ERC Starting Grant (“NanoArchive”) to develop a new trimodal hyphenated single particle platform consisting of an optical trap, a single particle Raman module and SP ICP-TOFMS. He plans to employ this new technology to pinpoint and characterise particles cycled through our atmosphere with previously unseen detail.

<https://orcid.org/0000-0003-3880-9385>



**Asst. Prof. Tea Zuliani** is a research associate at the Trace Elements Speciation Group of the Department of Environmental Sciences, Jožef Stefan Institute, Ljubljana, Slovenia, and an associate professor at the Jožef Stefan International Postgraduate School. She obtained her joint PhD in analytical chemistry at the Faculty of Chemistry and Chemical Technology of the University of Ljubljana, Slovenia, and at University of Pau and the Adour Region, France.

Her main research area is inorganic analytical chemistry of the environment and biological systems. The emphasis is on the development of analytical methods for trace element speciation and isotope ratio determination of non-traditional elements in environmental and biological samples, like speciation of organotin compounds, chromium, zinc, and nickel in different environmental samples, and application of stable isotope ratios of non-traditional elements in environmental, geological, provenance, archaeological and human studies.

<https://orcid.org/0000-0002-8367-876X>



Wednesday 11<sup>th</sup> September 2024

## Session 1

Keynote speaker 1

### The occurrence and drawbacks of two-phase aerosol transport upon ablation of soft biological matrices using nanosecond laser ablation-inductively coupled plasma-mass spectrometry

**Thibaut Van Acker**<sup>1</sup>, Tom Van Helden<sup>1</sup>, Kristina Mervič<sup>2</sup>, Ivan Nemet<sup>3</sup>, Johannes T. van Elteren<sup>2</sup>, Sanda Rončević<sup>3</sup>, Martin Šala<sup>2</sup>, Frank Vanhaecke<sup>1</sup>

<sup>1</sup>Department of Chemistry, Atomic & Mass Spectrometry – A&MS Research Group, Ghent University, Campus Sterre, Krijgslaan 281-S12, Ghent, Belgium. <sup>2</sup>National Institute of Chemistry, Hajdrihova 19, Ljubljana, Slovenia. <sup>3</sup>Department of Chemistry, Faculty of Science, University of Zagreb, Horvatovac 102a, Zagreb, Croatia

#### Abstract

Over the last decade, the development of novel low-dispersion ablation cells and highly efficient aerosol transport systems have boosted the analytical performance of laser ablation-inductively coupled plasma-mass spectrometry (LA-ICP-MS) regarding fast elemental mapping of solid samples. With single pulse response (SPR) profiles reaching sub-ms duration and thus, approaching the peak profiles typically encountered in single particle-ICP-MS upon detection of individual metallic nanoparticles.<sup>1,2</sup> The maximum achievable pixel acquisition rate depends on the duration of the SPR profiles and with high-end ArF\* excimer-based lasers capable of firing laser pulses up to 1 kHz repetition rate, acquisition rates up to 1,000 pixels/s can be achieved with low-dispersion setups. The SPR profiles do not only depend on the instrumental setup but also highly depend on the sample matrix, hardness and density, as well as the laser energy density and spot size since these parameters will determine the ablation yield. Recently, it was observed that SPR profiles are also element specific upon ablation of C-based materials, such as biological tissue and polymers.<sup>3</sup> Some elements are partially transported in particulate and gaseous phase, resulting in bimodal peak profiles. Therefore, the pixel acquisition rate needs to be reduced significantly relative to other elements, that are predominantly transported in particulate phase, to avoid smearing effects in the elemental maps.

1 T. Van Acker et al., *J. Anal. At. Spectrom.*, 2021, **36**, 1201–1209.

2 C. Neff et al., *J. Anal. At. Spectrom.*, 2022, **37**, 677-683.

3 T. Van Helden et al., *Anal. Chim. Acta*, 2024, **1287**, 342089.



## The application of LA-ICP-MC-MS for quantified, high spatial resolution imaging of Pb-Pb isotope ratios in ferromanganese crusts

Nathan Westwood<sup>1</sup>, Amy Managh<sup>1</sup>, Matthew Horstwood<sup>2</sup>, David Douglas<sup>3</sup>

<sup>1</sup>Loughborough University, Loughborough, United Kingdom. <sup>2</sup>British Geological Survey, Nottingham, United Kingdom. <sup>3</sup>Elemental Scientific Lasers LLC, Huntingdon, United Kingdom

### Abstract

Low limits of detection, near-full mass range coverage, and wide linear dynamic range of inductively coupled plasma-mass spectrometry (ICP-MS) combined with in-situ sampling by laser ablation (LA) provides a powerful tool for chemical mapping. Recently, there has been a proliferation of advances in both LA and ICP-MS instrumentation, as well as the introduction of accessories which have improved the interfacing between the two. These developments were predominantly driven by demand for high spatial resolution, higher throughput imaging in the biosciences which traditionally use time-of-flight or quadrupole ICP-MS platforms. Comparatively less attention has been paid to characterising these technologies for quantified imaging of geoscientific samples, particularly for multi-collector (MC)-ICP-MS systems.

This study focuses on the application of modern LA-ICP-(MC)-MS technology for high precision imaging of discrete Pb-Pb domains in ferromanganese crusts. Elemental and isotope ratio data were acquired using 193 nm LA systems, coupled to a MC-ICP-MS using low dispersion, high-efficiency transport accessories (*e.g.*, DCI, TwoVol2- and TwoVol3- ablation chambers). Parameters were adjusted between experiments such that image quality, data quality, and sample throughput were collectively optimised.

The results focus on the detailed characterisation of several Pb isotope ratio imaging methods for complex samples previously unapproachable by earlier generation technology. Identification and quantification of the uncertainty components inherent to data of this nature has been performed, along with documentation of the capability of modern map interrogation tools (*e.g.*, regions of interest and transects) for the extraction and representation of data directly from LA-ICP-(MC)-MS images.



## The effect of histological processing on indigenous elemental content and distribution in breast tumour tissue sections

Amy Lovejoy<sup>1,2</sup>, Alexander Morrell<sup>3</sup>, Alexander Griffiths<sup>3</sup>, Piotr Golda<sup>3</sup>, Evie Wren<sup>1</sup>, Kay Dawson<sup>1</sup>, George Lacey<sup>1</sup>, Charles Coombes<sup>1</sup>, Mark Rehkamper<sup>1</sup>, Rebekah Moore<sup>1</sup>

<sup>1</sup>Imperial College London, London, United Kingdom. <sup>2</sup>Institute of Cancer Research, London, United Kingdom. <sup>3</sup>King's College London, London, United Kingdom

### Abstract

Laser-ablation (LA)-ICP-MS has advanced significantly for studying biological elemental distributions. With matrix-matched standards and time-of-flight (TOF) technology, most elements in the periodic table can now be quantified at high spatial resolution. However, the impact of sample processing on indigenous metal content and distribution remains unclear. Formalin-fixed paraffin embedding (FFPE) is the preferred preservation technique for clinical samples, as it maintains tissue morphology and molecular components such as DNA.

This investigation aimed to determine if and how FFPE alters Zn and other elemental distributions. Snap-frozen breast tumour samples (n=3) were divided, with half undergoing FFPE and half processed frozen (FF). All samples (n=6) were sectioned and analysed via TOF and triple-quadrupole LA-ICP-MS at 10 µm resolution. Adjacent sections were histologically stained for high resolution microscopy to aid elemental image analysis. Formalin was sampled before and after sample fixation. The xylene and ethanol used to de-wax sections were also sampled. All solutions were analysed via triple-quadrupole ICP-MS.

The LA-ICP-MS data indicate that zinc concentrations in paired FFPE and FF sections remained comparable. Whilst one formalin solution appeared contaminated prior to fixation, metal leaching from the other two was minimal (including zinc, with 0.13-1.15ng/g increase). The direction of metal transfer during the dewaxing procedure was inconsistent, but the lacking gradation across the sections indicate that metals are not mobilised during processing, leaving the indigenous distributions intact. The current evidence suggests that the advantages of FFPE in terms of maintaining tissue integrity, availability and easy storage outweigh the risks of leaching and contamination.



**“Please sir, can I have some more?” – more elements, more dynamic range, more pixels, more samples! Getting the most out of time of flight ICP-MS and kHz laser ablation systems.**

Philip Shaw, Ariane Donard

Nu Instruments, Wrexham, United Kingdom

Abstract

The latest laser ablation systems from both ESL and Teledyne Photon Machines can ablate some sample types at 1kHz and fully resolve each lasershot’s signal to baseline count-rates. To make full use of this capability an ICP-MS must be able to store data to disk at a faster rate than the ablation, cover a significant range of elements to allow signal normalisation and be capable of measuring a wide range of count rates.

This presentation will describe the technical challenges of asking for more and use application examples in geology, biochemistry and materials science to show what is possible with the current instrumentation from Nu Instruments.



## Overcoming High-Complexity ICP-MS Tasks

David Price

PerkinElmer, Seer Green, United Kingdom

### Abstract

In the diverse realm of ICP-MS analysis, challenges span a spectrum of complexity. While some analytical paths offer a straightforward journey, others present formidable obstacles that demand expert navigation and innovative approaches.

This presentation will delve into the intricacies of high-complexity ICP-MS tasks, illuminating potential pitfalls and unveiling strategies to overcome them.

Join us as we explore how cutting-edge techniques and advanced instrumentation are revolutionising our ability to extract meaningful results from even the most demanding analytical scenarios.



## **Aerosol or liquid? A comparison of different dilution strategies for high-matrix ICP applications, including new automation approaches to reduce manual tasks in the lab.**

Raimund Wahlen

Agilent Technologies, Stockport, United Kingdom

### Abstract

The traditional approach to analyse high-matrix samples by ICP-MS has been to dilute samples in a liquid diluent – often with very high dilution factors to reduce Total Dissolved Solids (TDS) to less than 0.2%. Whilst this is a simple and fairly practical approach, it has a number of drawbacks such as additional analyst time, manual tasks and plastic waste, and potential for dilution errors or contamination.

Agilent first introduced fully-automated aerosol dilution capabilities for ICP-MS in 2009, with the High Matrix Introduction system (HMI), which allowed analysts for the first time to run much higher TDS samples (up to 25%) directly, without any prior liquid dilutions. This approach allows labs to improve their efficiency and reduce sample preparation tasks for previously challenging applications like routine seawater/brine analysis or high-throughput soil/waste-water testing, and avoid issues like diluent contamination or dilution errors.

Now Agilent are launching the first fully integrated liquid sample automation accessory for ICP-OES and ICP-MS that is developed and designed directly by the instrument manufacturer, in addition to the advanced aerosol dilution capabilities already available.

The new ADS-2 system has the highest level of hardware and software integration which provides benefits in terms of ease-of-use, unique functionality, and a single point of support for customers. In parallel with the hardware developments of the ADS-2 the instrument software has been updated with a host of novel features to provide a significant level of flexibility and functionality for customers looking to improve analytical workflows and reduce manual sample handling.



**Thursday 12<sup>th</sup> September**

**Session 2**

**Keynote speaker 2**

**Metal stable isotopes in the marine realm**

Dr Susan Little, Faculty of Engineering, Department of Earth Science & Engineering, Imperial College London, UK

Understanding the biogeochemical cycling of transition metals is important, because these elements are essential micronutrients, yet also often toxic at higher concentrations. Metal stable isotope measurements are a powerful tool to trace the sources and/or processes that control their distribution in the natural environment. The field of marine metal stable isotope geochemistry originated in the late 1990s, and has expanded dramatically over the last decade. Here, we briefly review the marine stable isotope cycling of several transition metals. Isotopic variability internal to the ocean is driven by a range of biogeochemical processes and their interaction with the physical ocean circulation. Mean whole ocean isotopic compositions are controlled by the isotopic composition of oceanic sources and fractionation into sedimentary sinks. The isotopic oceanic mass balance of each metal is reviewed, providing revised oceanic residence times estimates.



## Isotopic constraints on the biological and atmospheric controls of cadmium distribution in the Tropical North Atlantic

HUI XU<sup>1</sup>, Mark Rehkämper<sup>1</sup>, Yihang Huang<sup>1</sup>, Zijian Jia<sup>1</sup>, Rebekah E.T. Moore<sup>1</sup>, Arianna Olivelli<sup>1</sup>, Rob Middag<sup>2,3</sup>, Tina van de Flierdt<sup>1</sup>

<sup>1</sup>Imperial college London, LONDON, United Kingdom. <sup>2</sup>NIOZ Royal Netherlands Institute for Sea Research, Yerseke, Netherlands. <sup>3</sup>Centre for Isotope Research - Oceans, University of Groningen, Groningen, Netherlands

### Abstract

We systematically investigated the biogeochemical cycling of cadmium (Cd) and its stable isotopes within the Western Tropical North Atlantic (WTNA) to constrain the importance of local atmospheric deposition and remineralization. Seawater samples were collected at different depths from four sites in the WTNA and Cd was separated using a new and improved chromatographic procedure. High precision Cd isotope composition data ( $\delta^{114}\text{Cd}$ ) were then obtained via Multiple Collector ICP-MS. We found that atmospheric Cd contributes 20–80% of the total Cd to surface waters during the dust season; a factor previously underestimated in influencing Cd isotope compositions in the surface ocean. A box model was constructed to simulate the input and output fluxes in the surface water, constraining the atmospheric  $\delta^{114}\text{Cd}$  down to  $-0.4\text{‰}$ , showing a strong anthropogenic signal. Our study also highlights a 33–92% contribution of remineralization to the total Cd in the oxygen-depleted thermocline water outside the main Oxygen Minimum Zone, even with no obvious  $\delta^{114}\text{Cd}$  alteration. Finally, we used the isotope data to investigate the proportion of waters originating from the northern and southern hemispheres in deep waters, highlighting the preformed signals from different water mass source areas that dominate the distribution of Cd and  $\delta^{114}\text{Cd}$  in deep water. These findings highlight the complex interplay between atmospheric deposition, remineralization processes, and water mass origin in oceanic Cd distribution. I will discuss these new insights into the biogeochemical cycling of Cd and highlight the importance of considering both natural and anthropogenic influences in marine Cd isotope studies.



## **Effect of different weathering processes on the adsorption of arsenic, cadmium, chromium and lead on polyethylene, poly(ethylene terephthalate), polypropylene and poly(vinyl chloride) microplastics**

Bamikole Osungbemiro, Christine Davidson, John Liggat

University of Strathclyde, Glasgow, United Kingdom

### Abstract

In recent years, research has focused on understanding how microplastics host and transport potentially toxic elements (PTEs) in the aquatic environment. However, there is a considerable knowledge gap to be filled.

This study investigated the effect of laboratory-simulated photo-weathering (PW), thermal weathering (TW) and mechanical weathering (MW) on the adsorption of arsenic, cadmium, chromium and lead on polyethylene, poly(ethylene terephthalate), polypropylene and poly(vinyl chloride). The weathering microplastics were sampled and analysed weekly by Fourier transform infrared (FTIR) spectroscopy for 10 weeks. Batch adsorption experiments were carried out with virgin and weathered microplastics using 500 µg/L analyte solutions at pH 7.5 with agitation for 24 h at 170 rpm. The concentrations were determined by inductively coupled plasma mass spectrometry (7700X ICP-MS instrument, Agilent, Cheadle, UK).

The FTIR spectroscopy detected the presence of carbonyl groups in polyethylene and polypropylene after exposure to UV light, indicating photo-oxidation had occurred. The mean concentrations of metals adsorbed on virgin microplastics were 0.8 – 2.5 µg/g for arsenic, 2.3 – 3.1 µg/g for cadmium, 6.4 – 14.3 µg/g for chromium and 6.3 – 8.0 µg/g for lead. Weathered microplastics adsorbed higher concentrations of all PTEs than virgin microplastics following the order PW > MW > TW.

This highlights the influence of ageing in enhancing the capacity of microplastics to adsorb and transport PTEs. Further work will investigate the factors influencing the desorption of PTEs from both virgin and weathered microplastics.



**Winner of the Phil Ribby Award 2022  
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**A novel, robust field-sampling method for preserving mercury species associated with waters related to artisanal gold mining**

David King<sup>1,2</sup>, Michael Watts<sup>1</sup>, Elliott Hamilton<sup>1</sup>, Robert Mortimer<sup>3</sup>, Mike Coffey<sup>2</sup>, Marcello Di Bonito<sup>2,4</sup>

<sup>1</sup>British Geological Survey, Nottingham, United Kingdom. <sup>2</sup>Nottingham Trent University, Nottingham, United Kingdom. <sup>3</sup>York St John University, York, United Kingdom. <sup>4</sup>Università di Bologna, Bologna, Italy

**Abstract**

Mercury (Hg) is imported to Kenya for use in artisanal and small-scale gold mining (ASGM) at the rate of 6-45 tonnes per year and significant portions are released to the environment through mining activities. However, the ability to measure and identify Hg species in environmental matrices, particularly aqueous samples such as river waters, is challenging due to poor availability of technologies to provide representative Hg measurements. Concentrations of Hg species significantly decrease in water samples within 1 week of sampling if not preserved appropriately, lost predominantly to headspace and container materials. Current preservation methods are inadequate for field use, particularly in challenging environments such as ASGM sites. This leads to under-representation of Hg emission and toxicity in waters, used around ASGM sites for drinking, agriculture, and aquaculture.

Therefore, a robust method was necessary to provide measurements at sufficiently low Hg concentrations. The method must be sensitive, to provide useful public health and environmental regulatory information, and require non-hazardous and cost-effective materials.

A novel field-based solid-phase extraction method was developed to preserve Hg species from water samples for 4-weeks after sampling, avoiding interspecies conversion from field-collection to measurement, and is applicable in challenging environments such as artisanal gold mining (ASGM) sites in low-income countries. Both inorganic and methylated species were preserved and recovered >90% from water samples after 4-weeks of storage (n=5). Water and sediment samples were collected from rivers around ASGM sites to examine pollution of Hg species from mining activities and demonstrate effective assessment for environmental and human health.



## Speciation of mercury in sediments using high performance liquid chromatography hyphenated to inductively coupled plasma-mass spectrometry and a thermo-desorption technique

Abayneh Ambushe, Dipuo Precious Kgabi

University of Johannesburg, Johannesburg, South Africa

### Abstract

Speciation of Hg in sediments serves as a vital tool for assessing water quality since the actual toxicity, bioaccumulation and reactivity of Hg depend on its chemical forms. In this study, microwave assisted acid digestion and ultrasonic extraction methods were used to achieve a safe, simple and fast method for quantification of total Hg and Hg species in sediments, respectively. Total concentrations of Hg in sediment samples were determined by inductively coupled plasma-mass spectrometry (ICP-MS). Separation of the two species of Hg (methyl mercury [MeHg]<sup>+</sup> and inorganic Hg [Hg(II)]) by high performance liquid chromatography (HPLC) hyphenated to ICP-MS was achieved in less than 10 minutes using an isocratic elution with a mobile phase containing 0.4% L-cysteine, 0.05% 2-mercaptoethanol, 0.06 M ammonium acetate and 5% methanol. The accuracy of the method was confirmed and a percentage recovery of 86% was achieved. The Hg(II) concentration was found to be in the range of 38.4 to 89.05 ng/g and 34.8 to 57.3 ng/g in low and high flow seasons, respectively. The concentration of [MeHg]<sup>+</sup> was ranged from 0.702 – 4.5 ng/g and 0.5 to 2.5 ng/g in the low and high flow seasons, respectively. A thermo-desorption technique using a Zeeman direct Hg analyser was also used to quantify Hg in sediments and thermally speciate Hg to investigate the behaviour of Hg release from sediments. The sediment samples revealed the presence of different thermo species of Hg, most of which were associated with humic acid and/or iron oxides.



## An unconventional approach to the determination of oxygen isotope ratios in water using inductively coupled plasma – tandem mass spectrometry

Shaun Lancaster, Johanna Irrgeher, Thomas Prohaska

Montanuniversität Leoben, Leoben, Austria

### Abstract

Oxygen is one of the elements widely considered to be “unmeasurable” by plasma-based mass spectrometric techniques due to its high background, low ionisation potential, and multitude of interferences on each isotope. As part of the Unconventional Research funding call from Land Steiermark, Austria, we began to take the first steps towards making the unmeasurable measurable by developing a method for the determination of oxygen isotope ratios in water using inductively coupled plasma – tandem mass spectrometry (ICP-MS/MS). As the technique utilizes a mass filter before the reaction cell, only interferences with the same mass-to-charge ratio as the target isotope of oxygen need to be considered. Nitrous oxide, oxygen, hydrogen, ammonia, and helium cell gases were investigated to mitigate interferences from hydrides of oxygen and nitrogen, as well as doubly-charged interferences from argon and sulphur. Additionally, matrix suppression effects were investigated in order to be able to correct for differences in matrix salt loads.

Initial isotope ratio measurements were conducted using MilliQ water standards spiked gravimetrically with  $^{18}\text{O}$ -labelled water, the ratios of which agreed well with the calculated isotope ratios however with notably high uncertainties (bias: +1.2 ‰, uncertainty:  $\pm 2.3$  ‰). The developed methodology was then validated using water reference materials certified for  $\delta^{18}\text{O}/^{16}\text{O}$ . Although the uncertainties obtained using the ICP-MS/MS approach currently cannot compete with existing methods for determinations of oxygen isotope ratios, this study acts as a promising proof-of-concept for further developments in this field, where knowledge gained could be carried forward to future applications using plasma-based mass spectrometry approaches.



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## Session 3

Keynote speaker 3

### Gaining new perspective on the nano- and microscale: Combining elemental mass spectrometry and optical methods to characterise single particles

Prof. Dr. David Clases, University of Graz, Universitätsplatz 1, 8010 Graz, Austria

Nano- and microparticles are increasingly produced and emitted into the environment. Unfortunately, we continue to face difficulties to study their behaviour which are dependent on size, molecular and atomic composition as well as on number concentrations. This is anchored in the elusive nature of small particles and the requirement for very different analytical strategies to retrieve comprehensive and coherent information on a single particle level. As such, we fail to understand basic traits and their implications for human and environmental health. The development and maturation of single particle inductively coupled plasma – mass spectrometry (SP ICP-MS) set a paradigm shift for the tracing and characterisation of particles. However, the pure “elemental” perspective provided through SP ICP-MS also obscures our vision at the nano-scale and we are blind for a considerable number of particles as well as properties. This presentation will showcase new strategies to enable a comprehensive molecular and elemental characterisation of single particles (SP). Through the on-line coupling of two-dimensional optical traps, SP Raman spectroscopy and SP ICP-TOFMS, it becomes possible to carry out non-target screenings, to decipher the molecular and elemental composition of individual entities as well as to determine number concentrations and size distributions. The presentation will detail the underlying considerations and strategies and focus on new instrumentation, its hyphenation and future potential.

Literature:

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R. Gonzalez de Vega, T. E. Lockwood, L. Paton, L. Schlatt, D. Clases, “Non-target analysis and characterisation of nanoparticles in spirits via single particle ICP-TOF-MS”, J. Anal. At. Spectrom. (2023), 38, 2656-2663, (10.1039/D3JA00253E)



## **Biomonitoring for respirable crystalline silica: the determination of Si-containing particles in exhaled breath condensate using single particle inductively coupled mass spectrometry.**

Elizabeth Leese, Graeme Hunwin, Samantha Hall, Jackie Morton

HSE, Buxton, United Kingdom

### Abstract

Biological monitoring is a useful way of determining overall exposures to chemical substances; however, in the case of respirable crystalline silica (RCS), this has not been possible in conventional biological matrices. Previous research at HSE has shown that it was possible to detect silicon-containing particles in exhaled breath condensate (EBC) samples using single particle inductively coupled mass spectrometry (spICPMS) in a small number of quarry workers, and at that time the method had a particle size detection limit of around 300 nm.

In more recent work presented here we will describe the advances in the methodology and the results from exhaled breath condensate samples (n=30 workers) collected from three different UK workplaces with potential RCS exposures. Control samples were also collected for comparison (n=11 controls). The analytical advances include moving to using an ICP tandem MS for better specificity with an improved sample introduction system. This has increased the size range detection of silicon-containing particles, allowing measurements in the size range of 100-2000 nm, in a one minute acquisition. We have also standardised the EBC sampling by collecting the same volume of exhaled air (50L) from each volunteer. Static air/bulk samples were also collected to allow the size distribution and concentration of RCS to be determined in each workplace.

This improved methodology offers a viable biomonitoring method for a range of workplaces and has the potential to inform information about the efficacy of respiratory protective equipment and control measures in the workplace, complementing occupational hygiene.



## **When is a particle of interest? Single particle time of flight ICP-MS as a tool to determine particle numbers and true compositions.**

Philip Shaw, [Ariane Donard](#)

Nu Instruments, Wrexham, United Kingdom

### **Abstract**

The composition of a nanoparticle allows researchers to compare the behaviour and impact of natural, engineered and incidental nanoparticles (NPs) in the environment and biological systems. Bulk analysis techniques can determine the presence of NPs and the overall composition but it is only by examining the composition of each particle and comparing the distributions of composition to the flux of particles present, that inferences can be made about the impact of artificial particles compared to naturally occurring ones. The accurate measurement of particle numbers of each composition is a critical analytical requirement which can only be met by time of flight ICP-MS when considering metal containing particles. When the particles are completely unknown, time of flight ICP-MS is to the only realistic method to screen samples for non-target specific measurements. This presentation will describe the challenges of measuring individual particle content and processing the large quantity of data arising from routine analysis.



## Revisiting Single-Particle ICP-Mass Spectrometry (SP-ICP-MS) Approaches For Micro/Nano Quantification of Discrete Entities

Antonio Bazo, Eduardo Bolea-Fernandez, Ana Rúa-Ibarz, Maite Aramendía, Martín Resano

University of Zaragoza, Zaragoza, Spain

### Abstract

Micro- and nano-particles (MNPs) exhibit distinct size-dependent properties as compared to their larger-scale counterparts. Therefore, obtaining reliable information on the size of MNP populations is crucial for various fields, including environmental monitoring, food, and life sciences, among others. While several analytical techniques have already been used for the size determination of MNPs, single-particle inductively coupled plasma-mass spectrometry (SP-ICP-MS) has been identified as an emerging technology that can provide comprehensive information on thousands of MNPs in a short timeframe. Despite its first application in 2003, challenges remain in the data treatment of fast temporally resolved signals and the circumvention of matrix effects in SP-ICP-MS analysis.

To date, various approaches have been proposed to correlate the intensity or transit time of single events with their corresponding particle mass and size, highlighting (i) transport efficiency-dependent methods, (ii) transport efficiency-independent methods, and (iii) time-based approaches. This presentation systematically evaluates such methodologies for micro/nano quantification (sizing), aiming to identify and summarize their strengths and weaknesses, thus helping to identify their preferred areas of application. The performance of these methods was experimentally assessed using model MNPs, targeting both small (20-70 nm) metallic AuNPs and large (80-1000 nm) non-metallic SiO<sub>2</sub>MNPs.

Additionally, different setups and operation methodologies have been used for the simultaneous monitoring of MNP samples and ionic or NP spikes, so that the impact of the matrix on the characterization of such MNPs can be adequately corrected for. This presentation will also discuss the implementation of these approaches, along with their respective advantages and disadvantages.



## A fish tissue reference material certified for Ag nanoparticles? Progress so far.

Rob Clough<sup>1</sup>, Nathaniel Clark<sup>2</sup>, Adam Laycock<sup>3</sup>, Lenka Korbelová<sup>4</sup>, Jiří Herman<sup>4</sup>, Richard Handy<sup>2</sup>, Rachel Smith<sup>3</sup>

<sup>1</sup>Plymouth Atomic Mass Spectrometry Facility, School of Geography, Earth and Environmental Sciences, University of Plymouth, Plymouth, United Kingdom. <sup>2</sup>School of Biological and Marine Sciences, University of Plymouth, Plymouth, United Kingdom. <sup>3</sup>Toxicology Department, Radiation, Chemical and Environmental Hazards Directorate, UK Health Security Agency, Harwell, United Kingdom. <sup>4</sup>Secondary Industrial School of Chemistry, Pardubice, Czech Republic

### Abstract

The development of suitable analytical methods for measuring nanomaterials in complex matrices is hampered by a lack of appropriate reference material. The aim of this study was twofold: Firstly, to develop in-house silver nanoparticle (Ag NP) fish tissue reference material (RMs) and secondly to explore existing fish tissue CRMs for the presence of naturally occurring Ag NPs. To create the RMs, a perfusion technique was used whereby the fish were euthanised and cut open ventrally to expose the heart. The test material of 200 mg L<sup>-1</sup> Ag NPs in 40 ml of heparinised 0.9% NaCl was injected into the cardiovascular system through the base of the ventricles. Following perfusion, the fish gills and liver were collected, freeze dried and homogenised by milling. Three NRCC CRMs, DORM-4, DOLT-5 and TORT-2 were also analysed as part of this work. Samples were solubilised with either aqueous CaCl<sub>2</sub> and TMAH or a proteinase K solution followed by analysis by single particle inductively coupled plasma mass spectrometry (sp-ICP-MS). The results of these experiments will be presented and they show the suitability of the perfusion technique for creating an in-house RM. For example in liver the mean particle size was found to be 75 ± 2.1 nm and in gill 81 ± 3.3 nm. For the three CRMs Ag particles were detected in TORT-2, with the particle size being 28 ± 2.0 nm.



## PRECISE QUANTIFICATION OF METAL UPTAKE IN CELLS BY SINGLE CELL ICP-MS

Philip Holdship<sup>1</sup>, Megan Teh<sup>2</sup>, Michalina Mazurczyk<sup>2</sup>, Huei-Wen Chuang<sup>2</sup>, Andrew Armitage<sup>2</sup>, Jon Wade<sup>1</sup>, David Price<sup>3</sup>, Robert Hilton<sup>1</sup>, Hal Drakesmith<sup>2</sup>

<sup>1</sup>Department of Earth Sciences, University of Oxford, Oxford, United Kingdom. <sup>2</sup>Medical Research Council Translational Immune Discovery Unit, MRC Weatherall Institute of Molecular Medicine, University of Oxford, Oxford, United Kingdom. <sup>3</sup>PerkinElmer, Seer Green, United Kingdom

### Abstract

Metals are essential for the adequate functioning of all life. A key element is iron, which plays a vital role in many metabolic processes, such as oxygen transport by haemoglobin. Additionally, iron is vital for immunity against infection, where it is harnessed as an effective catalyst in activated T-cells during periods of infection<sup>1</sup>. Iron deficiency anaemia is a condition that affects around 1.2 billion people worldwide and impairs many aspects of physiology, including immunity<sup>2</sup>. Its prevalence is amplified in low-to middle-income countries, where the combination of malnutrition and endemic diseases result in unfavourable fates of disease progression and mortality<sup>3</sup>.

Precise measurements of iron within individual T-cells may provide a new and insightful tool for immunological research, where it could provide a metabolism-related biomarker of cellular immunological status. Such studies have traditionally adopted bulk-digestion and measurement approaches, but the single resultant average value can be misleading if the population displays cellular heterogeneity, which may occur under conditions of iron deficiency. Here we utilise single cell ICP-MS to rapidly scan the metallomic profile of large cell populations (>200 cells/minute). We evaluate the method developments that are required to enable the precise determination of metal uptake into cells, from experiments conducted on both human and mouse lymphocytes. We demonstrate that this approach yields precise quantification of T-cell iron content through a physiological range.

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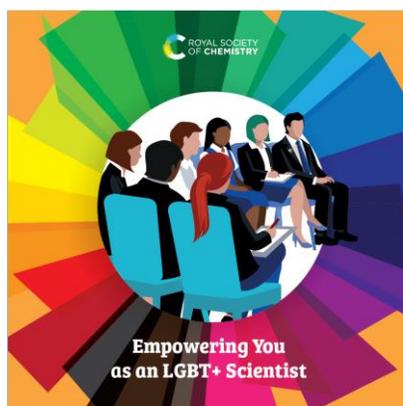
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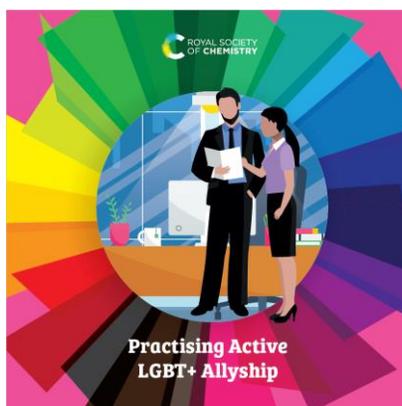
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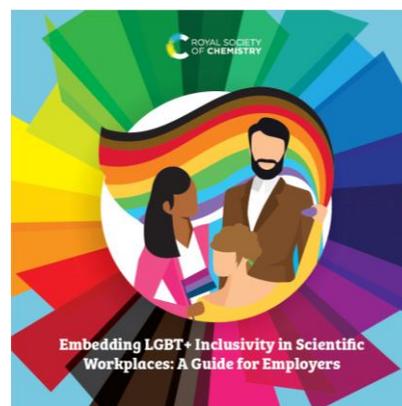
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**Friday 13<sup>th</sup> September**

**Session 4**

**Keynote speaker 4**

**High-precision analysis of non-traditional isotopes in environmental research**

Tea Zuliani<sup>1,2</sup>, Tjaša Žerdoner<sup>1,2</sup>, Majda Nikežić<sup>1,2</sup>

1. Department of Environmental Sciences, Jožef Stefan Institute, Ljubljana, Slovenia

2. Jožef Stefan International Postgraduate School, Ljubljana, Slovenia

The use of stable isotope ratios in the studies about elemental biogeochemical cycling and sourcing of materials (e.g. food, pollutants, historical remains, and artefacts) has undergone a transformative shift with the integration of non-traditional elements. While conventional light stable isotopes (C, H, O, N) have been pivotal in elucidating environmental processes, recent advancements extend the isotopic toolkit to include, for example, isotopes of strontium, lead, cadmium, and chromium and now play an essential role as tracers in Earth and environmental sciences. In parallel, advances in mass spectrometric instrumentation have markedly improved sensitivity and precision, facilitating the reliable detection of even the slightest fluctuations in the isotopic composition of elements with more than one natural isotope. However, despite these advancements, significant analytical challenges persist due to the diverse range of analyte/matrix combinations, concurrent matrix effects, spectral interferences, instrumental isotopic fractionation, and the lack of certified reference materials. The presentation will emphasize the versatility of non-traditional isotopes, highlighting their role in refining precision, expanding analytical capabilities, and deepening our understanding of interconnected systems. Furthermore, it will address the challenges of method development for accurate isotope ratio determination and the capabilities and limitations of various mass spectrometers.



## Isotope ratio measurements using ICP-MS/MS for source attribution of priority pollutants in air

Emma Braysher<sup>1</sup>, Jody Cheong<sup>1</sup>, Alex Dickinson<sup>2</sup>, Ben Russell<sup>1</sup>, Andrew Brown<sup>1</sup>, Richard Brown<sup>1</sup>

<sup>1</sup>National Physical Laboratory, Teddington, United Kingdom. <sup>2</sup>Royal Holloway University of London, Egham, United Kingdom

### Abstract

Heavy metals in airborne particulates are a serious health concern. Monitoring the concentrations of these metals in air and determining their sources allows for better control of toxic emissions and assessment of public exposure. NPL is using the latest generation ICP-MS instruments to expand its measurement capability for environmental pollutants. This presentation will outline the development and validation of a novel ICP-MS/MS method for isotope ratio measurements, comparing high-throughput methods with high-precision methods. It will identify a route to traceability for these measurements and their use for source apportionment of pollutants in ambient air.

Nickel is a pollutant of key concern in the UK as it is the only metal for which measured concentrations in one region have regularly exceed legislated limits. As polyatomic and tailing interferences make measurement of nickel in real samples difficult, interference removal techniques are discussed. Isotope ratio measurements of a nickel standard, using sample bracketing, are compared by MC-ICP-MS and ICP-MS/MS highlighting the strengths and weaknesses of each technique.

Although levels of lead in ambient air have fallen significantly in recent years, they are still higher than background levels. Improved source apportionment methods are vital to understand the origin of these pollutants in the air. The method developed has been applied to over 200 ambient air samples from across the UK. Variation of isotope ratios between different sites is discussed, as well as the implications for pollution contributions in different locations. This has been compared to an alternative high-precision isotope ratio method.



## Passive air quality investigation of leaves, moss and trees using Ion Beam Analysis techniques

Pierre Couture, Di Wu, Roger Webb, Vladimir Palitsin

Surrey Ion Beam Centre, Guildford, United Kingdom

### Abstract

Environmental conditions are of growing concern as large population are affected by climate change and pollution, an estimation of millions of people worldwide are dying from lower air quality [1]. Projects including living wall plant studied have been investigated to limit and improve air quality indoor and outdoor [1,2,3,4]. This project aims to explore the potential of plants, moss and trees as bio-indicators of environmental pollution. Quantification pollution indicator measured using Ion Beam Analysis (IBA) techniques; Rutherford backscattering (RBS), particle induced x-ray emission (PIXE). PTFE Air filters are used as supplementary samples to corroborate the findings from plant samples. This comprehensive approach also includes identifying potential pollution sources, thereby contributing to a broader understanding of environmental pollution dynamics in Guildford. The collection site locations were chosen to provide complementary information as NOx collection site are present along the motorway passing in the middle of Guildford. Sites along the railways were also chosen to have a wider representation of the possible pollution source in town. Other location sites were selected to function as controlled environment, location expected to have low level of pollution. In this presentation, we will show the latest results of qualitative and quantitative analysis of pollution indicators.

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## **Advancements in Multi-Element Speciation: A Novel Approach for the Identification of Chelating Compounds Using SEC-ICP-MS/MS and SEC-QTOF-MS with a Focus on Cadmium in Plant-Based Foods**

Julian Cardini, Jens Jørgen Sloth, Katrin Löschner

Technical University of Denmark, Kongens Lyngby, Denmark

### **Abstract**

The shift from meat- to plant-based diets necessitates understanding of heavy metals in plant-based foods. Cadmium, a toxic heavy metal, poses health risks. Research gaps persist in cadmium speciation, particularly its bioavailability and identification of cadmium binding compounds in plant-based foods.

This research presents an innovative methodology integrating SEC-ICP-MS/MS and SEC-QTOF-MS, for identifying Cd-binding compounds and simultaneous speciation analysis of multiple elements in plant-based foods. Sulphur and phosphorous play crucial roles in binding cadmium and can be used as markers for proteins and peptides. The presence of zinc, iron, and calcium might influence the bioavailability of cadmium.

The extraction process for cadmium was optimized across seven different matrices with varying protein content. This optimization yielded recoveries ranging from 2.3% to 72.3%, indicating strong cadmium binding to some matrices. Two size exclusion columns, with an optimal separation range of 600 kDa – 10 kDa and 7000 Da – 100 Da, were employed to separate the extracted compounds and optimized based on chromatographic peak resolution and analysis time. A 20% enhancement in resolution was achieved during the optimisation, with an analysis time of 60 minutes. For ICP-MS/MS-detection, the signal of the six elements was optimized based on the oxygen flow in the collision/reaction cell.

Clear differences in the cadmium binding patterns between different plant-based foods were observed. The established methodology represents a significant advancement of cadmium speciation in plant-based foods and can be applied in future bioaccessibility studies.



## Characterising chemical composition in brake wear using tandem inductively coupled plasma mass spectrometry (ICP-MS/MS)

Hau Lam Jody Cheong, Emma Braysher, Andrew Brown, Richard Brown

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### Abstract

The UK Health Forum estimates that illnesses linked to air pollution cost the NHS more than £2 billion in medical expenses each year and cause over 30,000 fatalities in the UK.<sup>1</sup> Non-exhaust emissions (NEEs) are becoming increasingly important as the number of electric vehicles on the road rises and exhaust emissions decrease as a result of legislation. Currently, there are no regulations for NEEs, which include brake wear, tyre wear, road surface abrasion and road dust resuspension, nor are there any standardised methods measuring their chemical compositions.

In this work, NPL has developed traceable measurement methods for brake wear using tandem inductively coupled plasma mass spectrometry (ICP-MS/MS). This presentation will outline the development of a novel sample preparation procedure and validation of an ICP-MS/MS method for measuring elemental components in brakes. Twelve metals have been studied and different instrument parameters, including interference removal modes, optimised to ensure measurements of sufficient precision. The uncertainty of the methods has been determined. The method has applied to measure heavy metals levels in various brake samples, obtained through different sampling techniques. The work has potential to provide properly validated data to benchmark air pollutants emissions inventory and improve knowledge of air quality in a Net Zero future.

Establishment of a representative sampling and a traceable measurement method allows improved comparison between different brake samples, leading to better control of NEEs. It will provide an evidence base for policy makers when defining legislative limits for road transport emissions.



## Measurement of cosmogenic Silicon-32 using inductively coupled plasma tandem mass spectrometry

Saskia Burke, Ben Russell

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### Abstract

The silicon chronometer (SINCHRON) project led by the Paul Scherrer Institute (PSI, Switzerland) identified  $^{32}\text{Si}$  as a cosmogenic radionuclide with the potential to be used for improved climate research to assess conditions on timescales of 100-1000 years. The implementation of  $^{32}\text{Si}$  is limited by poor agreement between historical half life values, ranging from 100-300 a. There is a need to improve and update the half-life through measurement of the same starting material using combined decay counting and mass spectrometric techniques.

Measurement of  $^{32}\text{Si}$  by inductively coupled mass spectrometry (ICP-MS) is challenging, due to the relatively short half-life, as well as interferences from  $^{16}\text{O}$  and  $^{32}\text{S}$ . This study investigates whether tandem ICP-MS/MS can overcome these interferences through the use of two quadrupole mass filters separated by a collision-reaction cell. Method development was carried out using stable Si and S standards, with the background monitored at  $m/z = 32$ . Multiple sample introduction systems were tested, with the ESI Apex Q providing the highest sensitivity. Multiple cell gases were tested for mass shifting of  $^{32}\text{Si}$ , with  $\text{NH}_3 + \text{H}_2$  effectively forming  $\text{SiNH}_2$ .

The optimised setup was tested on a  $^{32}\text{Si}$  standard, which successfully measured  $^{32}\text{SiNH}_2$  down to activity concentrations of 200 Bq/g (74 pg/g) with  $^{32}\text{S}$  and  $^{16}\text{O}_2$  not undergoing the same shift. This is the first known measurement of  $^{32}\text{Si}$  by ICP-MS/MS, further demonstrating the capabilities of this technique for online interference removal and expanding the number of radionuclides measurable by mass spectrometric techniques.



## Investigating inductively coupled plasma tandem mass spectrometry for measuring challenging radionuclides in steel samples as part of an interlaboratory comparison exercise

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National Physical Laboratory, Teddington, United Kingdom

### Abstract

Inductively coupled plasma tandem mass spectrometry (ICP-MS/MS) is increasingly used for measurement of radionuclides with a half life of  $\geq 10^2$  a. In some cases this approach offers rapid assessment compared to decay counting techniques, such as for uranium and plutonium isotopes. The online interference removal offered by ICP-MS/MS has also expanded the number of radionuclides that can be measured, to the extent that some of these can be considered almost routine (e.g. Strontium-90, Iodine-129 and Caesium-135/137).

There are several areas where measurement of radionuclides by mass spectrometry are beneficial. One is accurate assessment of the radiological composition of various materials in nuclear reactors undergoing decommissioning prior to waste sentencing. Steel is one such material, and was the focus of a recent international comparison exercise organised by VTT, Finland. A dissolved steel sample containing a range of medium and long-lived radionuclides of significant interest for waste characterisation was distributed to participants, including Chlorine-36, Calcium-41, Nickel-59, Nickel-63, Selenium-79, Molybdenum-93, Zirconium-93, Niobium-94. All of these radionuclides are potentially measurable by ICP-MS/MS, but have significant interferences that must be overcome to provide confidence in measurement.

This talk describes the development of ICP-MS/MS methods for measurement of radionuclides in steel samples, utilising online collision-reaction cell separation, supported by offline radiochemical separation when needed. Measurements were also compared to those made using radioactive decay counting techniques. This comparison is a valuable exercise in providing further evidence for the relative strengths and limitations of ICP-MS/MS for measurement of challenging radionuclides in complex matrices.



## Poster Abstracts



## 1. Role of High Accuracy Elemental Quantification Methods to Support Improved Comparability and Traceability for Magnetic Resonance Imaging

Ahmad Abukashabeh, Sarah Hill, Heidi Goenaga-Infante

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### Abstract

Quantitative MRI (qMRI), is becoming an important tool for clinicians, with the potential to replace physical biopsies e.g. iron overload in the liver. Metals such as Ni, Mn, Fe, mimic the T1 and T2 relaxation times which are key MRI parameters. Although considered a crucial diagnostic tool, MRI lacks consistency when comparing images obtained from different manufacturers or at different timepoints. This work describes a metrological approach to tackle this by developing well-characterised standards (known as phantoms), traceable to the International System of Units (SI), that can be used in typical clinical MRI facilities. This was achieved by combining gravimetric preparation and high accuracy elemental quantification, leading to SI traceable calibrants with low uncertainties (<1%, k=2). Phantoms were developed at 5 concentration levels and characterised by Isotope Dilution ICP-MS for Ni and Fe, with Exact Standard Matched calibration ICP-OES for Mn. Additionally, their long-term stability was assessed at 3-month intervals over 9 months at various temperatures (5°C, 18°C, 37°C, 60°C). Subtle trends were detectable due to the low uncertainties achieved by the high accuracy methods which are important to understand for the long-term viability of the phantoms. Furthermore, the phantoms were distributed to multiple clinical sites to collate data to further understand the differences between MRI systems on a larger scale and build models to overcome these effects. In conclusion, the use of high accuracy elemental analysis was essential to produce accurate and SI traceable measurements to underpin advances of MRI research and calibration for clinical diagnostics by qMRI.



## 2. Elemental Analysis in Yeast Cells and Selenium Enriched Yeast Cells by ICP-MS with Automated Micro-Flow Sample Introduction

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<sup>1</sup>Agilent Technologies, Santa Clara, USA. <sup>2</sup>Agilent Technologies, Stockport, United Kingdom

### Abstract

Technological advancements in ICP-MS hardware and software as well as optimized sample-introduction systems have opened up new approaches for single-particle and single cell analysis in recent years. In this study, an automated, micro-flow autosampler in combination with a high-sensitivity triple-quad Inductively Coupled Plasma-Mass Spectrometry (ICP-MS/MS) is used in the elemental analysis of nanoparticles and yeast cells. The sample introduction system is designed to deliver intact single cells or cell clusters to the plasma, while the ICP-MS offers high sensitivity and multi-elemental determination within the cell or cell cluster. The preliminary results from this study can potentially be applied to other applications, offering an easy and efficient way for high-throughput, multi-elemental single-cell analysis



### 3. A High Throughput Method for As Speciation in Urine

Olivia Cottam<sup>1</sup>, Adam Laycock<sup>1</sup>, Tim Marczylo<sup>1</sup>, Derrick Quarles<sup>2</sup>, Patrick Sullivan<sup>2</sup>, Paul Watson<sup>2</sup>, Nick Bohlim<sup>2</sup>

<sup>1</sup>Analytical Toxicology, Radiation, Chemical and Environmental Hazards Directorate, UK Health Security Agency, Harwell, United Kingdom. <sup>2</sup>Elemental Scientific Inc., Omaha, USA

#### Abstract

Arsenic toxicity is a significant public health concern due to its widespread environmental presence and association with various and severe adverse health outcomes including cancer, pulmonary and cardiovascular diseases, diabetes, and impaired cognitive development in children. Total arsenic measurement in urine is commonly employed to assess recent exposure since arsenic is primarily excreted via urine within 48 hours. However, arsenic toxicity differs significantly depending on its form. Inorganic As species, arsenate (As(V)) and arsenite (As(III)), are highly toxic and classified as Class 1 carcinogens. Their metabolites dimethylarsinic acid (DMA) and monomethylarsonic acid (MMA) still pose a risk, but are less toxic. Additionally, organic arsenic compounds like arsenocholine (AsC) and arsenobetaine (AsB), typically found in seafood, are considered to have low or no toxicity.

Here we present a rapid and automated method for determining arsenic speciation in urine using a prepFAST IC system from Elemental Scientific Inc, coupled to ICP-MS. This method allows for the separation of six arsenic species (AsB, DMA, MMA, AsC, As(III), and As(V)) in under two minutes. The capability for high-throughput arsenic speciation analysis is crucial for accurately assessing arsenic exposure, which can be used to enhance the accuracy of epidemiological studies and informs public health interventions aimed at reducing arsenic-related health impact



#### 4. Evaluating washing protocols for the determination of trace element concentrations in bird feathers by ICP-MS

Laura Crick<sup>1,2</sup>, Graeme Poole<sup>1</sup>, Emma Humphreys-Williams<sup>1,3</sup>, Jenny C. Dunn<sup>4</sup>, Jennifer L. Lavers<sup>5</sup>, Alexander L. Bond<sup>5</sup>

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##### Abstract

Feathers provide an excellent non-destructive biomonitoring tool for trace elements in the environment. Some analytical techniques can focus on individual elements, most notably mercury, but in many instances there is interest in a broader suite of elemental concentrations, particularly those of toxicological concern (arsenic, cadmium, mercury, lead). This is usually achieved through analysis of either whole or partial feathers using inductively coupled plasma mass spectrometry (ICP-MS).

For ICP-MS, samples must be first cleaned of external contamination, as the intrinsic elemental composition of the sample is of interest, and then digested into a solution. Cleaning removes particulate and organic matter that is not part of the feather itself, but which can contribute significantly to trace element concentrations if left in place, however to date there has been no consistent approach or evaluation to cleaning bird feathers for analysis by ICP-MS.

Using feathers from *Cygnus olor*, four commonly used cleaning methods were tested for their ability to remove V, Mn, Co, Cu, Zn, As, Cd, Hg and Pb. We demonstrate that a 2:1 mixture of chloroform and methanol is the most effective means of removing trace metals, including manganese and vanadium, whilst limiting additional contamination due to cleaning reagents.



## 5. Challenges of elemental impurity quantitation in high purity carbon in support of clean energy industries

John Entwisle, Sarah Hill, Heidi Goenaga Infante

LGC, Teddington, United Kingdom

### Abstract

High purity carbon and graphite are vital for advanced technologies as the world moves towards Net Zero. Uses include electronic vehicle batteries, fuel cells, wind turbines and hydrogen storage. Therefore, reliable trace element quantitation in these materials is essential, as impurities can impact product resilience and performance. Such methods will be invaluable to help industry comply with emerging regulations (e.g. EU Green Deal, Net Zero Industry Act, EU Regulation 2023/1542 Battery Lifecycles, etc.).

This poster describes methodology for the quantification of Al, B, Ca, Co, Cr, Cu, Fe, K, Mg, Mn, Na, Ni, P, S, Si, Ta, Ti, V and W in high purity carbon. In collaboration with a high purity graphite manufacturer, such elements were identified as essential to product quality. Method development and validation using NIST SRM 1635a Coal and BAM-S009 Graphite as quality control materials will be discussed. Sample preparation is based on microwave assisted digestion/extraction. The use of ICP-MS/MS implementing multiple reaction gas modes, enabled detection at the  $\mu\text{g}/\text{kg}$  level with fit for purpose LOQs obtained. The method was applied to real graphite samples from the manufacturer to assess the impact of modifications to the purification process. The results enabled process optimisation, therefore reducing energy requirements without affecting product quality.



## 6. Method validation for the determination of lead, cadmium and arsenic concentrations in human blood and the quantification of toxic metal exposure levels in two English cohorts.

Alex Griffiths<sup>1</sup>, Piotr Golda<sup>1</sup>, Alexander Morrell<sup>1</sup>, Ovnair Sepai<sup>2</sup>, Seeromanie Harding<sup>1</sup>, John Wright<sup>3</sup>, Seif Shaheen<sup>4</sup>

<sup>1</sup>King's College London, London, United Kingdom. <sup>2</sup>UKHSA, Oxford, United Kingdom. <sup>3</sup>Bradford Institute for Health Research, Bradford, United Kingdom. <sup>4</sup>Queen Mary University of London, London, United Kingdom

### Abstract

**Background:** Recently, the UKHSA public health action concentration (PHAC) for blood lead (Pb) concentration in pregnant women and children was reduced from  $\geq 10 \text{ ug dL}^{-1}$  to  $\geq 5 \text{ ug dL}^{-1}$ . The extent of chronic low-level exposure to Pb, as well as cadmium (Cd) and arsenic (As), and its contribution to adverse health outcomes remains unknown because of a lack of population-based UK data.

**Methods:** We have optimised and validated a method to accurately measure low toxic metal concentrations in whole blood and applied it to two English cohorts: the London-based Determinants of Adolescent Social well-being and Health (DASH) cohort, which obtained samples in 2013/14 from participants at 21–23 years old, and the Born in Bradford (BiB) cohort, which obtained samples from pregnant mothers and umbilical cord at birth in 2007–2010, and offspring in 2016–19 at 7–10 years old. Whole blood samples were digested for 60 minutes at 100 °C with  $\text{HNO}_3$  and  $\text{H}_2\text{O}_2$  and their toxic metal concentrations determined by ICP-MS using matrix-matched calibration standards.

**Results:** A total of 3,925 blood samples were analysed. Across both cohorts, toxic metal concentrations were log-normally distributed (median Pb, Cd and As concentrations were  $1 \text{ ug dL}^{-1}$ ,  $0.8 \text{ ug L}^{-1}$  and  $0.2 \text{ ug L}^{-1}$ , respectively). Importantly, ~1% of BiB exceeded the Pb PHAC while no DASH individuals exceeded the Pb PHAC for adults ( $\geq 10 \text{ ug dL}^{-1}$ ).

**Conclusions:** These data will be used to investigate associations between low-level toxic metal exposure and socio-demographic status, ethnicity, and health outcomes in these two cohorts.



## 7. Key considerations for the determination of metal contents in e-waste highlighted through inter-laboratory comparison

Shaun Lancaster<sup>1</sup>, Eskil Sahlin<sup>2</sup>, Marcus Oelze<sup>3</sup>, Markus Ostermann<sup>3</sup>, Jochen Vogl<sup>3</sup>, Valérie Laperche<sup>4</sup>, Solène Touze<sup>4</sup>, Jean-Philippe Ghestem<sup>4</sup>, Claire Dalencourt<sup>5</sup>, Régine Gendre<sup>5</sup>, Jessica Stammeier<sup>6</sup>, Ole Klein<sup>7</sup>, Daniel Pröfrock<sup>7</sup>, Gala Košarac<sup>8</sup>, Aida Jotanovic<sup>8</sup>, Luigi Bergamaschi<sup>9</sup>, Marco Di Luzio<sup>9</sup>, Giancarlo D'Agostino<sup>9</sup>, Radojko Jaćimović<sup>10</sup>, Melissa Eberhard<sup>1</sup>, Laura Feiner<sup>1</sup>, Simone Trimmel<sup>1</sup>, Alessandra Rachetti<sup>1</sup>, Timo Sara-Aho<sup>11</sup>, Anita Roethke<sup>12</sup>, Lena Michaliszyn<sup>12</sup>, Axel Pramann<sup>12</sup>, Olaf Rienitz<sup>12</sup>, Johanna Irrgeher<sup>1</sup>

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### Abstract

Electronic waste streams are an important source of large quantities of critical raw materials that underpin our society. As such, the European Commission has set new targets for recycling electronic waste in order to achieve a circular economy and reduce dependence on imports from other countries. One of the current major issues is the difficulty faced in analysing the wastes and quantifying the metal contents – a key step in determining the correct recycling pathways and in estimating the economic value of the waste stream.

As part of the MetroCycleEU project, an inter-laboratory comparison (ILC) was conducted between 10 research institutions across Europe on printed circuit board (PCB), light emitting diode (LED), and lithium ion battery (LIB) materials. Each institute provided multiple analyses of the materials, covering a range of x-ray fluorescence (XRF) and inductively coupled plasma (ICP) based methods. Additionally, instrumental neutron activation analysis was carried out as the “gold standard” analytical technique.

The results of the study clearly highlighted key aspects that affect measurement quality – In particular the limits of detection, interferences, and sample preparation. This work will detail the general trends observed from the ILC and suggest best practices for good quality measurements of electronic waste materials.



## 8. Evaluation of a novel quantitative blood sample collection device, Capitainer B50 card for heavy metals analysis

Jinkang Zhang, Adam Laycock, Tim Marczylo

Analytical Toxicology, Radiation, Chemical and Environmental Hazards Directorate, UK Health Security Agency, Harwell, United Kingdom

### Abstract

Dried blood spots (DBS) are widely used for quantification of blood analytes due to the ease of sampling and low-cost relative to venous blood. Accuracy of conventional DBS for quantitation of metals is however hampered by poor control over volume of blood sampled due to the haematocrit effect which determines the spread of sample on DBS and incomplete sample loading. Alternative quantitative blood sample collection devices have been developed to address these issues. In this study, we compared the quantification of blood Pb, Cd, As, and Cu using Capitainer B50 card (B50), conventional DBS card (Whatman 903 card) and whole blood (WB, as a benchmark). Recovery ratios of measured metals of certified blood samples from B50 were very good (range: 88% - 144%), while conventional DBS has significant variations of recovery ratios (range: -58% - 909%). Concordance correlation coefficient (CCC) analyses showed that B50 has excellent agreement with WB (Pb: CCC=0.995, Cd: CCC=0.998, As: CCC=0.930, Cu: CCC=0.936), while the same analysis confirms that conventional DBS have larger variation and poor consistency with WB. However, the detectable/quantifiable background levels of metals in B50 (e.g. Pb:  $1.02 \pm 0.32$  ng per disc of B50) may limit the application of B50 in blood metals analyses of low level samples. In summary, the improved performance of B50 in this study suggest it is more appropriate for quantitative blood sample collection for metals analysis, especially for screening of high-level metals exposures where costly phlebotomist-led WB collection, transportation and storage are prohibitive.



## 9. Lead Isotope Ratios to Identify Sources of Lead Exposure in Children

Adam Laycock<sup>1</sup>, Simon Chenery<sup>2</sup>, Elizabeth Marchant<sup>1</sup>, Helen Crabbe<sup>1</sup>, Ayoub Saei<sup>3</sup>, Ekaterine Ruadze<sup>4</sup>, Michael Watts<sup>2</sup>, Giovanni Leonardi<sup>1</sup>, Tim Marczylo<sup>1</sup>

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### Abstract

Lead (Pb) exposure in Georgian children is a significant public health concern, with a 2019/20 national survey revealing that 41% of children aged 2-7 years had blood lead concentrations (BLCs) greater than the blood lead reference value (BLRV) of  $\geq 5 \mu\text{g dL}^{-1}$ . This study aimed to determine total Pb concentrations and Pb isotope compositions in blood and environmental samples to identify probable sources of Pb exposure and guide intervention measures. Thirty-six children with BLCs above the BLRV were recruited, and environmental samples including spices, paint, soil, dust, flour, tea, toys, milk, and water were collected from their households. Total Pb and Pb isotope ratio determinations were performed using ICP-MS, and cluster analysis was utilized to identify significant sources of Pb. BLCs ranged from 2.5 to 39.9  $\mu\text{g dL}^{-1}$ , with many spice, paint, dust, and soil samples exceeding Georgian reference values. Isotope ratio analysis indicated that some spice and dust samples were most comparable to blood, while soil and paint samples were the most isotopically distinct from blood Pb. Cluster analysis suggested that adulterated spices were the most significant source of Pb exposure. The use of lead chromate pigments in spices to enhance color and weight is a documented practice in other countries. Identifying spices as a significant Pb source has informed authorities about spice adulteration practices, leading to targeted interventions. Further surveys are planned to assess changes in exposure sources and BLCs in Georgian children, ensuring the effectiveness of public health measures.



## 10. *In situ* zinc in breast cancer

Amy Lovejoy

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### Abstract

Zinc (Zn) is an essential metal, found in about a tenth of human proteins, with important roles in all of the body's systems. Therefore, unsurprisingly, diseases such as cancer are associated with changes to Zn balance (homeostasis). Many studies have found increases or decreases in zinc in blood serum and tissue samples associated with cancer. Such changes in Zn homeostasis have been attributed to the role of specific metalloproteins. In this poster, I show how I am investigating the main causes of overall Zn dyshomeostasis associated with breast cancer, using laser ablation ICP-MS, transcriptomics and machine learning; linking the *in situ* concentrations of Zn in different cells and tissues with different metalloproteins associated with breast cancer progression.



## 11. Elemental bioimaging of breast cancer tissues by LA-ICP-MS

Alexander Morrell, Alex Griffiths

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### Abstract

Triple-negative breast cancer (TNBC) is highly aggressive and challenging to treat. Metallomic profiling of cancerous tissues has received significant interest for diagnostic purposes as one-third of all enzymes and proteins contain a metal component.

Here, we have access to a unique tissue collection from TNBC positive patients before neoadjuvant chemotherapy (NACT) and clinical data relating to their response to treatment. Serial sections from these tissues obtained for imaging modalities are used for metallomic imaging by laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) and protein/ cell expression using a large panel of lanthanide tagged antibodies in imaging mass cytometry. These data show that metallomic imaging of endogenous metals important in cancer aetiology are correlated with the underlying cell/ protein expression. These correlative relationships are essential to move away from observational based interpretation of metallomic data and drive towards mechanistic understand of metals in relation to biology and disease.

Finally, we explore how time-of-flight based technology (Vitesse, Nu instruments) can eliminate the need of serial sections for this analysis. Typically, the lower mass range (mass <79) are filtered in imaging mass cytometry system to improve sensitivity of lanthanides, but key endogenous markers cannot be detected. By employing the time-of-flight, the entire mass range can be detected and correlations between endogenous metals and lanthanide tags can be measured simultaneously on a single tissue section. This removes the intrinsic variation caused by using serial sections and artefacts associated with registration. The benefits and challenges associated with employing this new strategy will be presented.



## 12. Quantifying zinc concentration and distribution in breast tissues via LA-ICP-MS and machine learning

Rebekah E. T. Moore<sup>1</sup>, Yifei Lin<sup>1</sup>, Alex Griffiths<sup>2</sup>, Amy Lovejoy<sup>1</sup>, Cristina Buenaventura Realingo<sup>1</sup>, R. Charles Coombes<sup>1</sup>, Mark Rehkämper<sup>1</sup>, Alex Morrell<sup>2</sup>

<sup>1</sup>Imperial College London, London, United Kingdom. <sup>2</sup>King's College London, London, United Kingdom

### Abstract

Zinc (Zn) is a structural or functional component of thousands of proteins and hundreds of enzymes and as such has been associated with multiple hallmarks of cancer. However, due to its many physiological functions, it is still unclear what its dominant roles in disease progressions are. Previous work has shown that 'normal' breast tissue contains less Zn than benign and malignant tumours and that the Zn in tumours is isotopically lighter than normal adjacent tissue (NAT).

Despite revealing significant differences, the bulk concentration and isotope results also revealed significant heterogeneity. To investigate this further, a subset of the same tissue samples were sectioned for *in situ* concentration analysis. One section from each was H&E (hematoxylin and eosin) stained, to image morphology, whilst adjacent, untreated, sections were used for laser ablation (LA)-ICP-MS. Calibration pico-gels were analysed alongside the samples, to enable quantification.

This poster presents elemental images with two spatial resolutions (35 and 2-3  $\mu\text{m}$  laser spot sizes). Zinc, magnesium, manganese, iron and copper were imaged on whole tissue sections at the lower spatial resolution. Targeted sections were chosen for higher resolution imaging to determine whether Zn concentrates more in the cells or extracellular matrix. Images clearly showed that Zn concentrates more in the cancerous regions and Zn distribution within benign and malignant NATs are different. QuPath was used alongside a convolutional neural network to further analyse the H&E-stained and elemental images, to enable quantification of elements in different cells (cancer, immune and epithelial), and stroma, at both resolutions.



### **13. Cone orifice diameter and ratio and its effect on dry plasma magnetic sector ICP-MS**

Claire Richards, Amy Managh

Loughborough University, Loughborough, United Kingdom

#### **Abstract**

In laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) analysis, the sampler and skimmer cone orifice sizes can significantly affect signal quality. The selection of the right set of cones for ICP-MS can influence factors such as sensitivity and background noise. Larger cone orifice sizes can increase sensitivity, but also background noise and the rate of oxide formation. Conversely, signal using smaller orifices may not be large enough to resolve from background noise. Can differing size orifice ratio also influence signal intensity of elements with a range of different properties for optimisation of methodology?

In this study, sector field LA-ICP-MS was used to analyse a variety of cone sizes and cone ratios. These were compared to standard sets and previous literature that used different mass spectrometer types. During the investigation successful results lowered the background signal noise, increased sensitivity, and lowered detection limits while maintaining similar laser conditions. Experimentally, both soft and hard particles were tested. In this context, NIST reference glass was used as a hard particle source. Microdroplets of a multielement standard printed onto a gelatine sheet were used as a soft particle source. Oxide formation was also investigated to determine which cone sets to avoid when analysing elements prone to producing oxides during ICP analysis.

This poster will aim to address choosing the most appropriate set of cones for various applications.



## 14. Method Development of Bioimaging Using LA-ICP-MS and Evaluation of Metal Accumulation in Comparison with Immunostaining Technology

Yukako Shintani-Domoto<sup>1</sup>, Yuki Sugiura<sup>2</sup>, Tetsuo Kubota<sup>3</sup>, Glenn Woods<sup>4</sup>, Raimund Wahlen<sup>4</sup>

<sup>1</sup>Department of Diagnostic Pathology, Nippon Medical School Hospital, Japan. <sup>2</sup>Center for Cancer Immunotherapy and Immunobiology, Kyoto University Graduate School of Medicine, Japan.

<sup>3</sup>Agilent Technologies, Hachioji, Japan. <sup>4</sup>Agilent Technologies, Stockport, United Kingdom

### Abstract

Bioimaging is widely used to visualize the presence or absence of certain tissues, cells, and low-molecular-weight compounds. Laser Ablation - Inductively Coupled Plasma - Mass Spectroscopy (LA-ICP-MS) can provide localization information of elements on solid samples. Therefore, bioimaging techniques using LA-ICP-MS have been developed to investigate the distribution of metals on thin sections. In this study, multi-element analysis on thin sections was demonstrated by using the Agilent 8900 ICP-QQQ or 7900 ICP-MS equipped with an ESL 213 Laser Ablation System (Elemental Scientific Lasers LLC (ESL)). Argon gas was used for sample carrier gas instead of He gas.



## 15. Exposure to nickel in UK workplaces

Jack Smith, Elizabeth Leese, Jackie Morton

HSE, Buxton, United Kingdom

### Abstract

Exposure to nickel in the workplace occurs in a wide number of occupational settings. Nickel compounds have been classified as a Group 1A carcinogen by IARC and are a known sensitiser. Metallic nickel is a suspected carcinogen with the IARC classification Group 2B. Therefore, it is vital that nickel exposure is kept to a minimum. The routes of exposure in a workplace can include inhalation, ingestion and dermal exposures. Biological monitoring, predominantly as the determination of nickel in urine samples, is routinely used to assess exposure. However, there is no UK guidance value for nickel in urine to assist with interpretation of results.

In this project, a current reference range for nickel was established in urine samples (n=100) from unexposed persons. Trends in urinary nickel results from 1996-2023 were also investigated from UK workers from results contained within the HSE Biological Monitoring database. Analysis of the worker data shows that a reduction in exposure over the last decade has been observed, with a P90 level of 25.4  $\mu\text{mol/mol}$  creatinine in 2014 (n=502) compared to 13.7  $\mu\text{mol/mol}$  creatinine in 2023 (n=1632). The aim of this data analysis is to group the different workplace types to better assess exposures across UK industry and to inform whether the decrease in urinary nickel levels is a result of lower risk workplaces undertaking biological monitoring or whether controls in workplaces have been improving.

All the analysis was undertaken using ICPMS and quality assurance ensured using both certified reference materials and participation in GEQAS.



## 16. Application of spectroscopy in food analysis

Volodymyr Vykhodtsev

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### Abstract

Spectroscopy is a powerful tool in the field of food analysis, allowing for quick, accurate and non-destructive analysis of the chemical composition and structure of various food products. This article considers modern spectroscopy methods, including infrared (IR) spectroscopy, ultraviolet and visible (UV-VIS) spectroscopy, nuclear magnetic resonance (NMR), as well as mass spectrometry. Their use to determine the quality, safety and authenticity of food products, as well as the detection of falsifications, are discussed. Particular attention is paid to the possibility of these methods to assess the content of proteins, fats, carbohydrates, vitamins and minerals in products. Examples of successful use of spectroscopic methods in the analysis of dairy products, meat, vegetables and fruits are presented. Conclusions are drawn about the prospects for the development of spectroscopy in the context of improving the efficiency and reliability of food quality control.



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