ABSTRACTS OF 67TH ICASS

I001

MICROWAVE DIGESTION AND ICP-MS FOR RELIABLE TRACE ELMENTAL ANALYSIS IN SHELLFISH. **Bob Lockerman**, Samuel Heckle, Marcy Harris, Layla Abu-Al-Halaweh CEM Corporation, 3100 Smith Farm Road, Matthews, NC 28104. (Bob.Lockerman@cem.com)

Shellfish are widely consumed due to their nutritional benefits, serving as rich sources of essential metals like iron, zinc, and magnesium. However, as bottom-dwelling organisms, they can accumulate environmental contaminants, including toxic heavy metals such as arsenic, cadmium, lead, and mercury, which pose significant health risks. Ensuring food safety requires thorough analysis of both beneficial and harmful elements. This study evaluates trace metal concentrations in various shellfish species, assessing both their nutritive and toxic elements. Microwave digestion is a critical sample preparation technique for accurate and reproducible trace metal analysis. Using ICP-MS analysis following microwave digestion, this method offers a rapid, efficient, and reliable approach to trace metal analysis in shellfish, supporting both nutritional assessment and food safety regulations.

I002

SELF-ORGANIZING MAPS FOR THE DETECTION AND CLASSIFICATION OF NATURAL NANOPARTICLES AND NANOPARTICLE SYSTEMS IN ENVIRONMENTAL NANOBIOGEOCHEMISTRY USING SINGLE PARTICLE ICP-TIME-OF-FLIGHT-MS. **Chad W. Cuss**, Laboratory for Environmental and Analytical Nanogeochemistry, Memorial University of Newfoundland (Grenfell Campus), Canada; Marc F. Benedetti and Mickaël Tharaud, Université Paris Cité – Institut de Physique du globe de Paris, CNRS, F75005 Paris, France; Carla Costamanga, Instituto de Química Física de Materiales, Ambiente y Energía (INQUIMAE), Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Argentina; Lucas Mesnard, Université PSL (Paris Sciences & Lettres), France. (ccuss@mun.ca)

Developments in nanotechnology have provided new instrumentation and analytical techniques which revolutionize our ability to measure the properties of nanoparticles (NPs), such as single-particle ICP-MS (spICP-MS). Originally developed to measure largely monodisperse and mono-elemental engineered nanoparticles (ENPs), adding a time-of-flight (ToF) mass analyzer to spICP-MS now facilitates multi-elemental measurements on the *millions* of polydisperse nanoparticles typically detected in each liter of natural waters. However, methods for processing and interpreting results are largely based on mono-elemental spICP-MS, prompting new questions:

- What is the best way to distinguish particle pulses from the natural background of metals caused by simple complexes and small molecules in e.g. a six-minute analysis, which produces more than four million data points for each isotope measured?
- What is the best way to characterize and compare highly heterogeneous and polydisperse natural nanoparticle systems (NNPS) for relating their properties to impacts in environmental roles?

These questions are at the core of emerging research in *environmental nanobiogeochemistry*.

After a brief introduction to environmental nanogeochemistry, self-organizing maps (SOM), and spICP-ToF-MS, this talk will describe advances and challenges in the application of SOM for detecting and characterizing the multi-elemental composition of NPs, distinguishing NNPS from different locations, and detecting multi-elemental ENPs in NNPS.

I003

UTILIZING A SWITCHABLE STATIONARY PHASE TO CONTROL SUPERCRITICAL FLUID CHROMATOGRAPHY (SFC) SEPARATIONS IN REAL TIME. **Kevin B. Thurbide** and Emmanuel A. Nai, Department of Chemistry, University of Calgary, 2500 University Dr. NW, Calgary, AB, T2N 1N4, Canada. (thurbide@ucalgary.ca)

Stationary phase development is important in SFC due to the impact it can have on separation selectivity. We have been developing a novel water stationary phase for SFC separations that utilizes carbon dioxide as the mobile phase, displays a normal phase separation pattern, is compatible with the universal flame ionization detector, and can be used to separate mixtures of various types of analytes. While the CO_2/water interface is inherently acidic (pH~3) during normal operation, the water stationary phase pH can be rapidly switched to basic (pH~9) in seconds by adding base to the system hydration source. This can also be reversed in a similar way, thus forming a useful pH switchable stationary phase. When coupled with a conventional SFC column, this switch can greatly modulate the velocity of ionizable analytes, whereas non-ionizable analytes are not affected. As a result, analyte selectivity and resolution can be readily controlled during separations, which can greatly simplify complex mixture analysis in SFC by helping to separate target analytes from interfering matrix components. The general operating characteristics of the system are detailed, and some applications of its use are discussed.

I004

DIMER FORMATION CONFIRMED: CLARIFYING ALTERNATIVE DRIVERS CONTRIBUTING TO PHOTO-ENHANCEMENT IN BROWN CARBON PHENOLS DURING DIRECT PHOTOLYSIS. **Shakiba Talebian**, Xinyang Guo, Ran Zhao. Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada. (stalebia@ualberta.ca)

Brown carbon (BrC) absorbs light and influences climate, yet its photochemical aging remains unclear. As BrC undergoes UV exposure, its composition and optical properties change, affecting atmospheric radiative forcing. Water-soluble BrC in clouds and fog under UV radiation initially enhances light absorption, possibly due to monomeric phenols forming dimers. However, identifying these dimers in complex aerosols has been challenging, limiting our understanding of their climate impact.

This study provides the first conclusive identification and quantification of phenolic dimers and their link to photo-enhancement. High-resolution LC-MS was used to analyze BrC transformations under UV radiation, focusing on five BrC-related phenols. Vanillin was examined in detail, with its dimer (Divanillin) compared to a commercial standard using Orbitrap mass spectrometry. Dimer yield, quantified via LC-MS, peaked at 10% under UVB light at 5 minutes before decreasing due to degradation. However, dimer formation did not directly correlate with photoenhancement, suggesting other products contribute to increased light absorption.

By applying advanced analytical techniques, this study confirms dimer formation while demonstrating that alternative factors drive photo-enhancement. These insights improve climate models and air quality predictions by clarifying BrC transformation mechanisms and their atmospheric effects.

I005

SOLID-STATE NMR ANALYSIS OF CARBOHYDRATE STRUCTURE REVEALS THE DYNAMIC REMODELING MECHANISM FOR FUNGAL SURVIVAL. Isha Gautam[1], Malitha Dickwella Widanage[1], Qinghui Cheng[1], Jayasubba Reddy Yarava[1], Ankur Ankur[1], Faith Scott[2], Andrew S. Lipton[3], Frederic Mentink-Vigier[2], **Tuo Wang**[1]. [1] Department of Chemistry, Michigan State University, East Lansing, MI 48864, USA; [2] National High Magnetic Field Laboratory, Florida State University, Tallahassee, FL 23310, USA; [3] Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory, Richland, WA, USA. (wangtuo1@msu.edu)

Invasive fungal infections pose a significant threat to human health, with high mortality rates persisting despite treatment. The rise of drug resistance has driven efforts to develop novel antifungal agents that target the fungal polysaccharides. Despite decades of molecular and biochemical research, the organization and interactions of polysaccharides in fungal cell walls remain poorly understood due to the complexity of analyzing these components within intact cells. Here, we highlight three recent advances enabled by ^{13}C/^{15}N/^{1}H solid-state NMR and Dynamic Nuclear Polarization (DNP). In *Aspergillus*, we identified structural modifications that reconfigure the carbohydrate network, enhancing resistance to the antifungal drugs named echinocandins, which target β-glucan synthesis. In *Mucorales*, major contributors to COVID-19-associated co-infections, we characterized a chitin- and chitosan-rich cell wall structure. Nikkomycin, a chitin synthesis inhibitor, selectively disrupted a specific chitin-chitosan-β-glucan complex while leaving other chitin structures intact, explaining the reduced susceptibility of these pathogens to this antifungal class. Finally, ^{1}H-detection of *Candida albicans* and the multidrug-resistant *Candida auris* revealed similar overall cell wall architectures but distinct remodeling responses to caspofungin treatment. These findings establish a structural framework for understanding fungal stress adaptation and antifungal resistance, offering crucial insights for the development of targeted therapies that disrupt cell wall biosynthesis.

I006

PHYTOREMEDIATION OF ROAD SALT IMPACTED SOILS. **Barbara Zeeb**[1], Amanda Chiasson[2], Lyndsay Cartwright[3], [1]Dept. of Chemistry & Chemical Engineering, Royal Military College of Canada, 13 Crerar Crescent, PO Box 17000, Station Forces, Kingston, ON, Canada; [2]School of Environmental Studies, Queens University, Kingston, ON, Canada; [3]Watershed Planning and Ecosystem Science, Toronto Region Conservation Authority, Vaughan, ON, Canada. (zeeb-b@rmc.ca)

Soil and water salinization are growing global concerns, adversely affecting both natural habitats and agricultural lands. In Canada, over five million tonnes of salts are applied to roads each winter to reduce vehicular accidents. These salts have lasting effects in roadside ecosystems as the chloride retained in soils is gradually released, and contributes to year-round persistence of salts in surface- and groundwater. Traditional methods of salt remediation are often costly and labour intensive with negative impacts on the environment due to the generation of by-products, accelerated soil erosion, and degraded soil conditions. Native Canadian halophytes (i.e. salt tolerant plants) are being evaluated for their abilities to remediate salt-contaminated soils along salted roadsides. As a primary limitation of phytoremediation is the relatively long time scales required for this technology to be effective, plant-associated microbes are also being investigated to enhance (and potentially speed up) the phytoremediation process. Three years of in situ studies initiated in 2022 in the Greater Toronto Area (GTA) will be presented. Consideration for the disposal of the salt-laden plant biomass will also be discussed.

I007

DETERMINATION AND SPECIATION OF SELENIUM IN FISH FROM LAKES AFFECTED BY FORMER OPEN COAL MINES. **Hailey Yu**, Xiufen Lu, X. Chris Le. University of Alberta, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, University of Alberta, Edmonton, Alberta T6G 2G3, Canada. (haixia6@ualberta.ca)

Selenium occurs naturally in the environment, with most of it stored in selenium-rich minerals. Open coal mining generates waste, which releases selenium into waterbodies by weathering processes. Selenium contamination poses potential harm to fish inhabiting in the affected waterbodies. Our analyses of water and fish collected from lakes near open coal mines show that the total selenium concentration in fish is still high although the coal mines have been closed and the water quality has improved. However, it is not known what selenium species are present in the fish. Our current research focuses on identification and quantification of selenium species. Our method combines high performance liquid chromatography (HPLC) separation with inductively coupled plasma mass spectrometry (ICPMS) detection. The target selenium species include selenite (Se^{IV}), selenate (Se^{VI}), selenocystine (SeCys), methylselenocysteine (MetSeCys), and selenomethionine (SeMet). We have achieved baseline-resolution of these selenium species using anion exchange HPLC. ICPMS detection at m/z of 78 provides sensitive and specific detection of selenium. This research on speciation of selenium is important because the different selenium species have different chemical properties and biological effects. The concentration and speciation information obtained from this research is critical for assessing environmental impact and fish consumption advisory.

I008

RUTHENIUM SPECIATION DURING ACIDIFICATION OF ALKALINE SOLUTION USING A UV-VISIBLE FAST DETECTOR AND AN *IN-SITU* PROBE. **Mathis Leblanc**[1], Sarah Baghdadi[1], Alexandre Quemet[1], Jean Aupiais[2]. [1]CEA, DES, ISEC, DMRC, Univ Montpellier, Marcoule, France. [2]CEA, DAM, DIF, 91297 Arpajon, France. (mathis.leblanc@cea.fr)

Ruthenium is a highly radioactive and volatile fission product of interest in the context of nuclear fuel reprocessing R&D studies. Its radioactivity also benefits the nuclear medicine field. Taking into account its tendency to volatilize in oxidizing media, alkaline traps are often used to capture Ru vapors. An acidification of the samples or an alkalization of the standards is required to analyze an element by ICP-MS or ICP-OES of these alkaline solutions. However, this step leads to the precipitation of most of the Ru in solution, resulting in an incorrect quantification. This study aims to identify and quantify the acidification by-products and understand their formation mechanisms. A UV-Visible fast detector coupled to an *in-situ* probe monitors the existing Ru species at a millisecond scale. Thousands of spectra with large Ru-bands are obtained and then deconvoluted using a Multivariate Curve Resolution algorithm. Results indicate a two-steps reaction: the first one involving ruthenate (RuO_4^{2-}) and leading to perruthenate (RuO_4^-) and a Ru(V) precipitate; the second one involving the perruthenate and leading to the release of the same Ru(V) precipitate and the highly volatile ruthenium tetroxide (RuO_4). These analyses help to estimate the formation and kinetic constants of these reactions.

I009

WHAT CAN WE LEARN ABOUT BRAIN PROTEINS AND PEPTIDES BY USING BIOELECTROCHEMISTRY **Sanela Martic,** Department of Forensic Science, Environmental and Life Sciences Program, Trent School of Environment, Materials Science Program, Water Quality Center, Trent University, Peterborough, ON, K9L 0G2, Canada. (sanelamartic@trentu.ca)

Biolectrochemistry is a powerful analytical tool offering opportunities for new discoveries to be made in the field of peptide and protein biochemistry, which are often unobtainable using standard analytical methods. Using proteins on Au surfaces, we demonstrated that fundamental biomolecular interactions can be monitored using cyclic voltammetry and electrochemical impedance spectroscopy. We reported on using electrochemical methods for detection of protein-protein interactions, protein-ligand interactions, enzymatic catalysis, enzyme inhibition, and metallation while focusing on tau protein biochemistry.[1] The solution electrochemical studies provided information with regards to redox activity of metallo-peptide complexes and their relative stability. Bioelectrochemical methodologies were used to gain insight into various facets of protein and peptide biochemistry, and represent promising bioanalytical tools.

[1] A) Carlin, N., Martic-Milne, S. (2018). Anti-tau antibodies based electrochemical sensor for detection of tau protein. J. Electrochem. Soc.165: G3018-G3025. B) Jahshan, A., Esteves, J.O.V., Martic-Milne, S. (2016). Evaluation of ferritin and transferrin binding to tau protein. J. Inorg. Biochem. 162: 127-134. C) Trzeciakiewicz, H., Esteves, J.O.V., Carlin, N., Martic, S. (2015). Electrochemistry of heparin binding to tau protein on Au surfaces. Electrochim. Acta. 162: 24-30.

I010

DEVELOPMENT AND APPLICATION OF ZEEMAN-PERTURBED NQR SPECTROSCOPY TO STUDY HALOGEN BONDS IN SOLIDS. Alireza Nari, Mubassira Rahman, Patrick M.J. Szell, Volodymyr Semeniuchenko, and **David L. Bryce**, University of Ottawa, Ottawa, ON, Canada (David.Bryce@uottawa.ca)

One of the main benefits of ultrahigh applied external magnetic fields in solid-state NMR spectroscopy is the line-narrowing and concomitant increased resolution for half-integer spin quadrupolar nuclei. However, even at the highest available fields (e.g., 36 T series-connected hybrid magnet at the US MagLab), the observation via NMR of many strongly quadrupolar isotopes remains highly impractical or impossible. Nuclear quadrupole resonance (NQR) represents an appealing alternative technique because relatively sharp resonances may be obtained without the need for an external magnetic field. Two practical constraints we have encountered with pure NQR include difficulties in measuring the quadrupolar asymmetry parameter from simple one-dimensional measurements, and the inaccessibility of high-frequency (i.e., hundreds of megahertz) resonances of certain isotopes and transitions due to limitations of commonly available hardware. We describe here our recent work on the implementation of a modern version of Zeeman-perturbed NQR spectroscopy, where a tunable electromagnetic from an EPR spectrometer is used to generate spectral line shapes which depend on the quadrupolar coupling constant and asymmetry parameter. The method is applied to record $^{79/81}$Br and ^{127}I Zp-NQR spectra of a series of halogen bonded cocrystals featuring quadrupolar coupling constants of up to 2.3 GHz. These data are shown to correlate with the strength of the halogen bonds.

I011

MIXED COLLOIDAL STANDARDS WITH TRACE ELEMENTS FOR NANOPARTICLE ANALYSIS USING ASYMMETRIC FLOW FIELD-FLOW FRACTIONATION COUPLED TO INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Claire M. Churchill**[1], Salani U. Fernando[1], Isabelle A. M. Worms[2], Michaela Mühlbauer[3], and Chad W. Cuss[1]. [1]School of Science and the Environment, Grenfell Campus, Memorial University of Newfoundland, Corner Brook, NLL A2H 5G4, Canada; [2] University of Geneva, [3] Postnova Analytics GmbH (cmchurchill@mun.ca)

Asymmetric flow field-flow fractionation (AF4) coupled to inductively coupled plasma mass spectrometry (ICP-MS) has a range of applications in environmental nanogeochemistry, particularly to analyze different size fractions that correspond to different forms in environmental samples, e.g. small molecules and simple complexes < 300 Da, DOM-associated forms, small inorganic and larger inorganic forms. The size of these colloids is directly related to their mobility, reactivity, and potential toxicity. However, stable colloidal standards suited to the verification of AF4-ICPMS to analyze complex environmental samples are still to be developed. Standards for AF4-ICPMS allow comparisons of methods and results which facilitates consistency across laboratories. Thus, this presentation will discuss the development of a reproducible standard composed of an organic and inorganic colloid mixture with associated trace elements for AF4-ICPMS. The viability of a mixed colloid-trace element standard based on its stability over time will be discussed, along with the reproducibility of its production as determined by analysis using AF4-ICPMS. Colloid mixtures were filtered to obtain the <0.22, 0.45 and 1.2 µm fractions. Temperature, pH, and conductivity were measured and controlled to maintain reproducibility. Results from interlaboratory comparisons between labs in Canada, Switzerland and Germany will also be discussed.

I012

ANALYSIS OF PROTEINS AND EXTRACELLULAR VESICLES USING NOVEL BIOASSAY PLATFORMS. Rebecca Goodrum, Roshan Aggarwal, **Huiyan Li,** School of Engineering, University of Guelph, Canada (huiyanli@uoguelph.ca)

Extracellular vesicles (EVs) are nanoscale particles secreted from cells. EVs carry biomolecules such as proteins and nucleic acids that are very similar to their cells of origin, thus providing a useful tool for disease detection. Quantifying EVs and their protein concentrations can provide important information on health and diseases [1]. Classical EV and protein analysis technologies such as enzyme-linked immunosorbent assay (ELISA) and western blotting have limitations on assay sensitivity and multiplexing capability, unsuitable for disease biomarker discovery [2]. In this talk, I will present novel proteomic platforms that we have recently developed integrating nanomaterials into microscale bioassays. These platforms have been applied for EV and protein quantification, with improved assay sensitivity, scalability, and convenience compared to conventional methods. Complex biological samples such as blood plasma have been tested using these technologies, demonstrating their potential in measuring real patient samples. These advantages make these new technologies powerful tools in biomedical research. Potential applications include biomarker detection in complex diseases such as cancer and cardiovascular diseases.

[1] A. Bodaghi, N. Fattahi, A. Ramazani. Heliyon. 2023. E13323.
[2] N. Momenbeitolahi, T. Cloet, H. Li. Anal. Bioanal. Chem. 2021. 5995-6011.

I013

PAN-CANCER N-GLYCOPROTEOMIC ATLAS OF PATIENT-DERIVED XENOGRAFTS UNCOVERS FAT2 AS A THERAPEUTIC TARGET FOR HEAD AND NECK CANCERS.

Meinusha Govindarajan[1], Salvador Mejia-Guerrero[2], Shawn C Chafe[3], Shahbaz Khan[2], Wei Shi[2], Matthew Waas[2], Amanda Khoo[1], Lydia Y Liu[1], Vladimir Ignatchenko[2], Simona Principe[2], Lusia Sepiashvili[1], Nazanin Tatari[3], Chitra Venugopal[3], Petar Miletic[3], Maxwell Topley[3], Shan Grewal[3], Dillon McKenna[3], Maria-Jose Sandi[2], Nhu-An Pham[2], Alison Casey2, Hyeyeon Kim[1], Christina Karamboulas[2], Jalna Meens[2], Peter Bergqvist[4], Begonia Silva[4], Patrick Chan[4], Liza Cerna-Portillo[4], Jasmine Chin[4], Abilasha Rao-Bhatia[4], Ming-Sound Tsao[2], Rama Khokha[1,2], Susie Su[5], Wei Xu[2,5], David Goldstein[6], Laurie Ailles[1,2], Vuk Stambolic[1,2], Fei-Fei Liu[2], Emma Cummins[4], Ismael Samudio[4], Sheila K Singh[3], **Thomas Kislinger**[1,2]. [1]Department of Medical Biophysics, University of Toronto, Toronto, Canada; [2]Princess Margaret Cancer Centre, University Health Network, Toronto, Canada; [3]Centre for Discovery in Cancer Research, McMaster University, Hamilton, Canada; [4]adMare BioInnovations, Vancouver, Canada; [5]Dalla Lana School of Public Health, University of Toronto, Toronto, Canada; [6]Department of Otolaryngology-Head & Neck Surgery, University of Toronto, Toronto, Canada. (thomas.kislinger@utoronto.ca)

Cell surface proteins offer significant cancer therapeutic potential attributable to their accessible membrane localization and central role in cellular signaling. Despite this, their promise remains largely untapped due to the technical challenges inherent to profiling cell surface proteins. Here, we employed N-glycoproteomics to analyze 85 patient-derived xenografts (PDX), constructing GlycoPDXplorer – an in vivo pan-cancer atlas of cancer-derived cell surface proteins. We developed a target discovery pipeline to prioritize proteins with favorable expression profiles for immunotherapeutic targeting and validated FAT2 as a head and neck squamous cancer (HNSC) enriched surface protein with limited expression in normal tissue. Functional studies revealed that FAT2 is essential for HNSC growth and adhesion through regulation of surface architecture and integrin-PI3K signaling. Chimeric antigen receptor (CAR) T cells targeting FAT2 demonstrated potent anti-tumor activity in HNSC models. This work lays the foundation for developing FAT2-targeted therapies and represents a pivotal resource to inform therapeutic target discovery for multiple cancers.

I014 P

STRUCTURE AND BONDING OF NANO-SILVER: A THEORETICAL ANALYSIS.

Enoch Zhang, Andrew Walsh, Peng Zhang, Department of Chemistry, Dalhousie University, Halifax, NS, Canada. (peng.zhang@dal.ca)

Silver-based nanomaterials are promising materials for various biomedical applications. Understanding the structure-property relationship of nano-silver at atomic scale plays an important role toward developing high-performance functional materials towards these applications. In this poster presentation, a series of magic number silver nanoclusters with varied sizes and alloying composition are studied by quantum theoretical spectroscopy analysis. It is found that silver atoms at specific atomic sites such as vertex, edge and terrace surface site show significantly different bonding properties. When the size of the nano-silver is varied, the average electronic and bonding properties are found to be highly dependent on the cluster size and coordination environment. Finally, silver-gold alloy nanoclusters with well-defined core-shell structure are investigated and bonding properties of the silver-gold samples are compared with their silver counterparts to demonstrate the alloy effect on the structure and properties of nano-silver. These findings will be useful to better understand the structure-property relationship of nano-silver from the perspective of atomic site, cluster size and alloy bonding.

I015

X-RAY SPECTROSCOPY ANALYSIS OF NANO-ALLOYS. **Peng Zhang,** Department of Chemistry, Dalhousie University, Halifax, NS, Canada. (peng.zhang@dal.ca)

Synchrotron X-ray spectroscopy and associated techniques are powerful tools for in-depth analysis of atomic structure and electronic properties of catalysts. In this talk, the application of such techniques in the study of alloy nanostructures will be presented. Materials of interest include bimetallic single-atom-alloy catalysts and multi-element systems such as high-entropy alloys. It will be demonstrated that the X-ray spectroscopy techniques, together with associated experimental and computational methods, are very useful in illustrating how the atomic structure and electronic properties of the nanoalloys are correlated with their catalytic performance. The element-specific analysis of multi-metallic alloy systems using energy-tunable X-ray techniques is expected to become a future routine towards more completely understanding their structure-property relationships for catalytic applications.

I016

A LIPIDOMIC ARRAY FOR 10-SECOND DIAGNOSIS OF COMMIN SPINAL TUMOUR TYPES WITH PICOSECOND INFRARED LASER MASS SPECTROMETRY. Alexa Fiorante[1,2], Michael Woolman[1,2], David G. Munoz[3,6], Taira Kiyota[4], Lan Anna Ye[1], Yasmine Farahmand[1], Darah Vlaminck[1,2], Francis O. Talbot[1], Sunit Das[5,6], Sorcha Kellett[6], Christine Giuffrida[6], Gelareh Zadeh[1,5], Howard J. Ginsberg [3,5,6], Ahmed Aman[4,7] and **Arash Zarrine-Afsar** [1,2,5,6], [1] Princess Margaret Cancer Centre, University Health Network, 101 College Street, Toronto, ON, M5G 1L7, Canada; [2] Department of Medical Biophysics, University of Toronto, 101 College Street, Toronto, ON, M5G 1L7, Canada; [3]Department of Laboratory Medicine and Pathobiology, University of Toronto, 1 King's College Circle, Toronto, ON, M5S 1A8, Canada; [4] Ontario Institute for Cancer Research (OICR), 661 University Ave Suite 510, Toronto, ON, M5G 0A3, Canada; [5] Department of Surgery, University of Toronto, 149 College Street, Toronto, ON, M5T 1P5, Canada; [6] Keenan Research Center for Biomedical Science & the Li Ka Shing Knowledge Institute, St. Michael's Hospital, 30 Bond Street, Toronto, ON, M5B 1W8, Canada; [7] Leslie Dan, Faculty of Pharmacy, University of Toronto, 144 College St, Toronto, ON, M5S 3M2, Canada. (arash.zarrine.afsar@utoronto.ca)

Improving surgical outcomes for spinal neoplasms requires precise intraoperative diagnosis provided by neuropathologist on call as surveys of outcome data have suggested suitable extents (aggressiveness) of resection to improve survival for each neoplasm type. However, personalization of the extent of resection relies on subjective assessments wherein the depth of diagnosis depends on the experience of the (neuro)pathologist. Through a retrospective study of *n*=319 patient specimens we evaluated the utility of 10-second picosecond infrared laser mass spectrometry (PIRL-MS) for non-subjective diagnosis of major spinal tumour types. The sensitivity and specificity values of spinal tumour type diagnosis were (93±1)% and (97±2)%, respectively. This classification utilized n=41 cellular lipids including phosphatidylcholines, sphingomyelins, phosphatidylethanolamines, and ceramides whose identities were established using high-resolution tandem mass spectrometry. Furthermore, the accuracy of diagnosis was not influenced by the presence of new data not ‘seen’ by the model confirming the generalizability of the identified lipidomic array in rendering correct classification of spinal neoplasms. The identified lipids form a ‘molecular array’ for robust diagnosis of spinal tumours by non-pathologists in a manner similar to transcriptomic or methylomic arrays used to diagnose brain cancer types, albeit on a much faster timescale of seconds as opposed to hours.

I017

TACKLING CHALLENGING SAMPLES: ALTERNATIVE STRATEGIES FOR ELEMENTAL ANALYSIS USING ATOMIC AND MASS SPECTROMETRY. **Daniel L. G. Borges,** Universidade Federal de Santa Catarina, CFM – Chemistry Department, Florianópolis – SC, Brazil. (daniel.borges@ufsc.br)

Atomic spectrometry techniques are widely used and consolidated tools for elemental quantification. However, the techniques are known to be matrix-sensitive, which frequently demands time-consuming sample preparation. Our group has been devoted to developing simpler strategies to tackle a series of analytical challenges. Electrothermal vaporization / atomization using ICP-MS and high-resolution continuum source atomic absorption spectrometry has been extensively assessed as a tool for the introduction of solid samples (coal, geological samples, ceramic catalysts, polymers, etc.) either directly or as slurries, for the quantification of analytes as diverse as rare earth elements and halogens. Elemental speciation and fractionation analysis in multiphase oily sludge has also been carried out using mild extraction strategies and detection using either ICP-MS or atomic fluorescence spectrometry. The same assessment has been investigated using lab-made dielectric barrier discharge devices, which were miniaturized for the analysis of single drops with femtogram detection limits, as will be further discussed. Finally, the possibility of carrying out analyte-matrix separation based on photochemical vapor generation will be demonstrated, with applications based solely on a “dilute-and-shoot” approach. Overall, the examples should demonstrate that analytical challenges may be overcome with alternative sample introduction strategies and, quite often, minimum sample preparation.

I018

IMPACTS OF SALT TYPE ON SOLVENT-BASED PROTEIN PRECIPITATION: IMPLICATIONS FOR PROTEOMICS ANALYSIS BY MASS SPECTROMETRY. **Alan A. Doucette**[1], Ziheng Dang[1], & Jessica Nickerson[2]; [1]Department of Chemistry, Dalhousie University, 6243 Alumni Crescent, Halifax, NS B3H 4R2, Canada; [2]Allumiqs Corporation, 1344 Summer St., Halifax, NS B3H 0A8, Canada. (alan.doucette@dal.ca)

We previously demonstrated the critical importance of salt, or more specifically of ionic species to induce protein precipitation using organic solvents. We proposed that solvated cations and anions are coulombically attracted to residual protein charges, leading to ion pairing in lower dielectric strength solvents. This effectively neutralizes all protein charge, causing precipitation through hydrophobic attractions. Here, we address whether the *type* of salt matters. Certainly, some salts (*eg* $ZnSO_4$) require lower concentrations to induce precipitation vs other salts (*eg* $ZnCl_2$). $MgCl_2$ needs very little while $CuCl_2$ needs a lot; $ZnSO_4$ and Na_2SO_4 are intermediary, indicating critical roles for both the cation and anion. Our salt recovery trends do not align with the Hofmeister series nor other expected trends (charge, ionic radius…), lending the follow up – *why* does salt type matter? Next, we address whether salts preferentially precipitate proteins according to intrinsic protein properties (charge, size, hydrophobicity). This would bias recovery and MS-based proteome analysis. Alternatively, solvent precipitation could potentially be a desirable tool for proteome fractionation by class. A detailed proteomics analysis of precipitated proteins using various salts was completed, allowing a greater understanding of the role of salts for solvent-based protein precipitation and its implications on MS-based proteomics analysis.

I019 P

RARE EARTH ELEMENT ANALYSIS USING NEXION 5000 ICP-MS SYSTEM. **Sandeep Kumar**, Aaron Hineman, and Chady Stephan, PerkinElmer Scientific Canada ULC, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada. (Sandeep.Kumar@PERKINELMER.COM)

Due to diverse technological applications of rare earth elements (REEs), there is need for increase in geological exploration to find new REE deposits. Most of these technological applications of REE based devices are dependent on the purity of REEs, and although REEs occur naturally, they are usually at low concentrations. For this reason, having ICP-MS instrumentation which is able to deliver exceptional background equivalent concentrations (BECs) and detection limits (DLs) to support these ultra-trace measurements is desired. Another obstacle when analyzing REEs using ICP-MS with triple-quadrupole or multi-quadrupole functionality is the difficulty in removal of any on-mass oxides and polyatomics. To address these interferences, pure reaction gases, such as NH_3, is used to react with either the interference or the analyte ions in the collision/reaction cell to remove the interference. Therefore, having an instrument such as Nexion 5000 which can run pure reaction gases, such as ammonia, is highly advantageous. In this presentation, we will discuss methods using NexION® 5000 Multi-Quadrupole ICP-MS for the determination of trace rare earth element concentrations, and impurities in a high-purity rare earth oxide matrix. Data will be presented for several rare earth element impurities analyzed using Multi Quad mode and using pure reaction gases.

I020

ANALYSIS OF ORGANOMETALLIC COMPOUNDS AND METALLIC PARTICLES IN SPECIALTY GASES BY DIRECT INJECTION USING GAS EXCHANGE DEVICE (GED) COUPLED TO INDUCTIVELY COUPLED PLASMA-MASS SPECTROMETRY (ICP-MS). Sandeep Kumar, **Aaron Hineman**, and Chady Stephan. PerkinElmer Scientific Canada ULC, 501 Rowntree Dairy Rd, Woodbridge, ON L4L 8H1, Canada. (Aaron.Hineman@PERKINELMER.COM)

In this work, we will introduce the concept of Gas Exchange Device (GED) and how it is used to monitor organometallic compounds and metallic particles in specialty gases. GED-ICP-MS workflow eliminate the need for any off-line sample preparation making it the ideal tool for metallic impurities monitoring for in-process chemicals at delivery, distribution, and point of use in industries. Specialty gases for semiconductor and electronics industry range from the pyrophoric and/or toxic gases required for thin film deposition and doping, through to reactive and corrosive gases needed in different etching steps. Conventional method to test for metallic impurities in specialty gases utilizes the impinger of filters. However, these techniques are known to have limitations with respect to the impurities exchange to the liquid media, contamination during collection process, solubility of compounds, filter material suitability etc. These methods also require extended sample preparation and have issues with moisture sensitive gases. We present here gas direct injection, a technique that enables the direct analysis of a sample gas without the need to utilize an impinger. GED – ICP-MS offers a fully automated workflow for direct analysis. Two applications, carbon monoxide (CO) and hydrochloric gas (HCl), will be discussed comparing obtained results by GED-ICP-MS versus impinger.

I021

ASHING AND DIGESTION OF ENVIRONMENTAL MATRICES USING FOCUSED INFRARED HEATING FOR SAMPLE PREPARATION. **Tristan Bélanger**,[1] Nicolas Guérin,[2] Dominic Larivière.[1] [1]Department of Chemistry, Université Laval, Québec, Québec, Canada, G1V 0A6; [2]Canadian Nuclear Laboratories (CNL), Chalk River, Ontario, Canada, K0J 1J0. (tristan.belanger.1@ulaval.ca)

Environmental samples must be solubilised in acidic solutions to analyse elements of interests. The sample dissolution often requires ashing of the sample in a muffle furnace to remove the organic matter. The ashing process is time-consuming and tedious, which limits the number of samples that can be analysed. New ashing methods are needed. ColdBlock Technologies has recently developed an acid digestion apparatus based on focused infrared heating. The apparatus has infrared lamps that could be powerful enough to ash environmental samples. In this study, the capability of the ColdBlock device to ash samples rich in organic matter was studied. Sea fish, spinach leaves, and tomato leaves, with known amounts of Th-232 and U-238, were ashed and digested with the Coldblock apparatus. The chemical recoveries for Th and U were most of the time comparable to the traditional muffle furnace ashing method, but the samples were ashed considerably faster with the ColdBlock device (1,5 h instead of 8 h). Focused infrared ashing could be an interesting alternative to current ashing methods.

I022

DON’T LET IT GET UNDER YOUR SKIN: OPTIMIZATION OF CHITOSAN-BASED ARTIFICIAL SKIN MEMBRANES FOR INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS) BASED IN VITRO PERMEABILITY STUDIES OF TRACE ELEMENTS IN COSMETIC AND PERSONAL CARE PRODUCTS. **Nausheen W. Sadiq**, Lisa Tritz and Birhan Gezahegn, Mount Royal University, Department of Chemistry & Physics, 4825 Mount Royal Gate SW, Calgary, AB T3E 6K6, Canada (nsadiq@mtroyal.ca).

As cosmetic and personal care products are ubiquitous and often used daily, the determination of trace elements is imperative to ensure their safety. Through risk assessment studies, regulations to protect environmental and human health can be strengthened. Quantitative and qualitative risk assessments often involve in vitro and animal studies that evaluate exposure to individual elements. These studies may not account for multi-elemental exposure, chemical interactions, and exposure frequency. The development of in vitro study models for risk assessment of trace elements is important to address these shortcomings. ICP-MS was used to determine the concentration of trace elements (Al, V, Cr, Mn, Ni, Zn, As, Se, Cd, Hg, Pb) in commercially available cosmetics, several containing high levels of Cd, Hg and Pb! Using chitosan-based membranes, synthesized to mimic human skin, and 3D-printed diffusion cells, the concentrations of trace elements that permeate across the dermal layers were determined. The suitability of the membranes for this experiment in representing “real skin” were assessed by comparing them with Strat-M® membranes, the industry standard. The chitosan membranes are designed to offer a low-cost, biodegradable alternative, and help to accurately determine the risk associated with cosmetic and personal care products to human health.

I023

LASER-INDUCED BREAKDOWN SPECTROSCOPY (LIBS) TO MEASURE QUANTITATIVELY EXCHANGEABLE SOIL ELEMENTS. **Fanny Hernandez**[1], Maxime Magre[1], Marc Ramon[1], Matthieu Chazalon[2], Clotilde Aschero[2], Guillaume Desperrières[2], Matthieu Dubernet[1,2]. [1]Laboratoires Dubernet, 35, rue de la combe du meunier, 11100 Montredon des Corbières – France ; [2]Terra Mea 35, rue de la combe du meunier, 11100 Montredon des Corbières – France. (fanny.hernandez@dubernet.com)

Soil is an essential ecosystem providing food, biomass, regulating water, carbon and nutrient cycles. Accurate soil measurement is crucial to effectively addressing environmental challenges. Moreover, soil management in agricultural systems is crucial and depends on the knowledge of soil chemical, physical and biological properties. Conventional wet chemical methods are labor intensive and time consuming as it requires several techniques. Laser-induced breakdown spectroscopy (LIBS) as an alternative technique has already demonstrated promising results for the analysis of several soil parameters such as pH, texture, soil organic matter, total elemental analysis ... The aim of this study is to develop and validate a LIBS method to quantify exchangeable nutrient elements in soils using multivariate partial least squares regression method (PLS).

I024

AN OVERVIEW OF THE LIBS DEVELOPMENT AND LASER BASED APPROACHES FOR IMPROVING LIBS SENSITIVITY. **M. Sabsabi**[1], E. Soares de Lima Filho[1], P. Bouchard[1], A. Harhira[1], J. El Haddad[1], F. Vanier[1], D. Gagnon[1], I. ElHamdaoui[2], S. Selmani[2], F. Vidal[2], M. Constantin[3]. [1]Clean Energy Innovations Research Center, National Research Council Canada, 75 de Mortagne Blvd., Boucherville, QC J4B 6Y4 Canada; [2]Institut national de la recherche scientifique, Centre Énergie Matériaux Télécommunications, 1650 boul. Lionel-Boulet, Varennes, QC J3X 1P7, Canada; [3]Université Laval, Département de géologie et de génie géologique, 1065 Ave de la Médecine, Québec, QC G1V 0A6, Canada. (mohamad.sabsabi@cnrc-nrc.gc,ca)

Laser-Induced Breakdown Spectroscopy (LIBS) is a versatile analytical technique integrating multiple scientific disciplines, including laser-matter interaction, plasma physics, and spectroscopy. Unlike stationary plasma types such as inductively coupled plasma or arc plasma, LIBS utilizes a transient plasma, which has prompted extensive research over the past thirty years to enhance its sensitivity and performance. Recent advancements include the double pulse mode, the integration of LIBS with Laser-Induced Fluorescence (LIBS-LIF), known as LIBS-LIF, Resonant Enhanced LIBS (RELIBS), Resonant Laser Ablation (RLA), Resonant Laser Ablation assisted by Laser Induced Fluorescence RLA-LIF. These approaches hold promise for rapid, in situ analysis with minimal sample preparation, particularly beneficial for clean energy and environmental applications. The LIBS-LIF technique involves using an initial conventional laser to ablate the sample and create a plasma, followed by a second tunable laser that selectively excites the plasma, enhancing the emission of specific spectral lines. The presentation will cover significant research achievements in enhancing LIBS-LIF's quantitative analysis, with applications spanning environmental, agricultural, and mining sectors. It will also explore novel approaches to boost LIBS's sensitivity and analytical performance. Furthermore, the presentation will discuss the recent progress in LIBS technology, driven by advancements in pulsed lasers, detectors, and spectrometers, leading to increased adoption in diverse fields such as geology, planetary science, and food safety. The talk will highlight emerging strategies for improving LIBS sensitivity and its integration with other techniques, offering a forward-looking perspective on its future developments and potential applications.

I025

QUANTIFICATION OF NATURALLY-OCCURING RADIONUCLIDES IN FOOD BY ICP-MS/MS. **Dominic Lariviere**, Marie Roy, Laurie Martin, Department of Chemistry, Université Laval, Québec, QC G1V 0A6, Canada. (dominic.lariviere@chm.ulaval.ca)

Uranium, thorium, and radium-226 are naturally occurring radioactive elements that decay by emitting alpha particles. These radioisotopes are found in the earth's crust and contribute to natural radioactivity, including that which may be present in food. Among the different types of radiation, alpha particles pose the greatest risk once inside the human body.

As part of this project, we developed and validated analytical methods for the precise measurement of U, Th, and Ra-226 in the Canadian diet, bottled water and edible wildlife samples using ICP-MS. This presentation will highlight the analytical challenges and innovations involved in the rapid quantification of these radionuclides across various food matrices. The results were compared to maximum annual dose limits, confirming that the measured concentrations do not pose a health risk to consumers.

I026

BAYESIAN AND FREQUENTIST APPROACHES FOR DETERMINING MEASUREMENT ERROR MODELS FOR LC-MS PROTEOMICS & METABOLOMICS. **T.K. Karakach**[1,2], F. Bong F. [1,2], P.D. Wentzell[1,3]. [1]Laboratory of Integrative Multi-Omics Research, Department of Pharmacology, Dalhousie University, Halifax, NS B3H 4R2, Canada; [2]Beatrice Hunter Cancer Research Institute, Halifax, NS B3H 4R2, Canada; [3]Department of Chemistry, Dalhousie University, Halifax, NS B3H 4R2, Canada. (kararakach@dal.ca)

Liquid chromatography–mass spectrometry (LC-MS) is a cornerstone of modern proteomics and metabolomics, yet the resulting data are often complex and heterogeneous, necessitating robust statistical frameworks for interpretation. Generalized least squares models are frequently employed to assess the relationship between instrumental response (y_i) and biological covariates (x_p), under the null hypothesis that regression coefficients (β_j) are zero (i.e., $y_i = \beta_j x_p + \varepsilon_i$). These models assume normally distributed data and homoscedastic, independent errors ($\varepsilon_i \sim$ iid Normal). In practice, however, LC-MS data often violate these assumptions, and standard transformation methods may not adequately address issues such as error non-uniformity also known as heteroscedasticity. Here, we present a parametric approach for estimating variance functions in LC-MS data, developed through an experiment specifically designed to quantify measurement uncertainty and disentangle contributions from multiple sources of variability. We show that, under appropriate experimental design, total variance can be decomposed hierarchically as: $\sigma_{total}^2 = \sigma_{biol}^2 + \sigma_{tech}^2$, where $\sigma_{biol}^2 \gg \sigma_{tech}^2$, *i.e.*, the biological variance ($\sigma^2{}_{biol}$) dominating. Additionally, we characterize the multivariate error structure, identifying correlations among features, and introduce a model to capture this covariance structure, enabling accurate estimation of LC-MS measurement error with minimal replication. The derived error variance model, developed using both Bayesian and frequentist methods, facilitates data pre-processing that preserves the analytical relevance of low-intensity signals. This approach improves statistical modeling of LC-MS data by integrating realistic error structures, thereby enhancing the reliability of downstream quantitative analyses in proteomics and metabolomics workflows.

I027

ENHANCING OUR UNDERSTANDING OF VIROCEUTICALS USING AN OPTIMIZED MASS SPECTROMETRY-BASED LIPIDOMICS APPROACH. Joshua A. Roberts[1], Elena Godbout[2], Jocelyn A. Menard[1], Christopher N. Boddy[3], Jean-Simon Diallo[2,4], **Jeffrey C. Smith**[1,5,6], [1]Department of Chemistry, Carleton University, [2]Ottawa Hospital Research Institute, University of Ottawa, [3]Department of Chemistry and Biomolecular Sciences, University of Ottawa, [4]Virica Biotech, Ottawa, ON, [5]Institute of Biochemistry, Carleton University, [6]Carleton Mass Spectrometry Centre, Carleton University. (JeffCSmith@CUNET.CARLETON.CA)

Lentiviral Vectors (LV) are emerging tools for genetic therapies and novel cancer treatments with extremely large costs associated with their manufacturing and delivery. We have developed a rapid, robust, and sensitive untargeted lipidomics pipeline to analyze novel LV biotherapeutic products and demonstrate its utility on HEK 293T packaging cells and concentrated culture media containing LV. HEK 293T cells were cultured to confluence and divided into three populations: untreated, treated with a VSV G plasmid, or treated with all four plasmids coding the production of LV. Each population was left for 24, 48, and 72 hours before harvesting and analyzed in triplicate by HPLC-MS. 151 lipids were identified in HEK 293T packaging cells, 84 of which had fold changes with FDR-corrected $P<0.05$ compared to HEK 293T treated with media. It was found that fold changes with FDR-adjusted $P<0.05$ after VSV G expression and LV production were highly correlated ($R^2=0.89$). Concentrating LV in culture media led to the identification of 102 lipids, half of which were determined to be unique LV virion lipids after subtracting the media lipidome. Our approach can be readily used to study the lipid dynamics of large-scale LV production or applied to other viral vector platforms.

I028

COMBUSTION FURNACE ANALYSIS OF PLASTIC AND DERIVATIVE PRODUCTS: TECHNIQUES AND APPLICATIONS FROM PROCESSING TO DISPOSAL. **Bartosz Jasiak**, Scion Instruments Canada Ltd. (bartosz.jasiak@analytik-jena.com)

The widespread use of plastics necessitates precise analytical techniques to assess their composition, quality, and potential contaminants. In parallel, the growing concern over plastic waste highlights the need for robust detection and quantification methods due to its environmental and human health risks. This talk seeks to showcase techniques for the analysis of impurities from plastic products and derivatives, including pyrolysis oils, as well as wastewater contaminants. Sulfur and chlorine have presented unique difficulties with large variations in concentration and propensity for damage to the environment and machinery. Combustion furnace technology provides a reliable approach for analyzing mixed materials, particularly in determining carbon, nitrogen, sulfur, and chlorine content. These systems ensure high sensitivity, reproducibility, and compliance with regulatory standards. For this analysis, the multi EA 5100, multi EA 4000, and multi N/C TOC series products were utilized. Their automation capabilities, including self-cleaning injectors, matrix-adaptive combustion control, and intelligent monitoring functions, enhance efficiency while minimizing human intervention and contamination risks.

I029

LIPIDOMICS ANALYSIS REVEALS A DYNAMICS LANDSCAPE OF THE PATHOGENESIS OF *ACINETOBACTER BAUMANNII*: INSIGHTS INTO LIPID METABOLISM AND IMMUNE-INFLAMMATORY RESPONSES.

Stupak[1], Harris Greg[1], Sam Williamson[1], Rui Chen[1], H. Howard Xu[2], Wangxue Chen[1] and **Jianjun Li[1]**. [1]Human Health Therapeutics Research Centre, National Research Council Canada, 100 Sussex Drive, Ottawa, Ontario, K1A 0R6, Canada. [2]Department of Biological Sciences, California State University Los Angeles, Los Angeles, CA, USA. (jianjun.li@nrc-cnrc.gc.ca)

In this presentation, we present the application of NPLC-FAIMS-HRMS to analyze the serum lipid dynamics after *Acinetobacter baumannii* infection. The temporal profiles of serum lipids after *A. baumannii* inoculation were obtained for 4 h, 8 h and 24 h. We found an early and sustained decrease in PI 38:4 (18:0-20:4) species in the sera of infected mice as early as 4 h; whereas PI 34:1 (16:0-18:1). This discrepancy is due to the fact that phosphoinositides are an important class of signaling lipids and involved in host inflammatory and immune responses. At 8 h, the levels of 22 lipids were significantly decreased. This phenomenon may be explained by the fact that *A. baumannii* infection induces clinical symptoms within 8 h of infection, and lung tissue damage thereafter. The results from 24 h post inoculation animals indicate 28 species were increased and 28 species were decreased in the sera of infected mice at this time point. It is surprising that 11 PE and 7 PS species contain either AA (20:4) or DHA (22:6). Our findings reveal dynamic changes in the serum lipidome during *A. baumannii* infection, confirming that lipids play important roles in host inflammatory and immune responses.

I030

IMPACT OF LYSIMETER SELECTION ON POREWATER SAMPLING AND DISSOLVED TRACE ELEMENT DISTRIBUTION: IMPLICATIONS FOR ENVIRONMENTAL MONITORING.

Salani U. Fernando, Lakshman W. Galagedara, Manokararajah Krishnapillai, Chad W. Cuss**,** School of Science and the Environment, Memorial University of Newfoundland, Corner Brook, NLL A2H 5G4, Canada. (ksufufernand@mun.ca)

Accurate assessment of trace element (TE) distributions amongst small molecules and simple complexes (< ca. 300 Da), dissolved organic matter, and larger inorganic species in soil solutions is essential for understanding their mobility, bioavailability, and environmental impact. While the influence of sampling methods on TE concentrations is well recognized, their effect on TE distribution remains underexplored. This study investigates the impact of three lysimeter types, Rhizon, SPE20 nylon, and SiC, on the distribution of dissolved (< 0.45 µm) TEs in soil solutions from three distinct locations in Alberta and Newfoundland. The distribution of dissolved TE was analyzed using asymmetric flow field-flow fractionation coupled with inductively coupled plasma mass spectrometry (AF4-ICPMS). Key findings reveal that lysimeter material composition significantly affects TE measurements, primarily due to the sorption and leaching behaviors. Additionally, pore size variations can influence the collection of TEs, particularly those associated with nanoparticles and colloidal forms. Regional differences in soil chemistry also influence TE mobility and interactions with lysimeter materials. Understanding how sampling techniques influence TE distribution is vital for improving data reliability in soil studies, supporting sustainable land management, and enhancing environmental quality assessments.

I029

CE-MS METABOLOMIC AND LC-MS PROTEOMIC ANALYSES OF BREAST CANCER EXOSOMES REVEAL ALTERATIONS IN PURINE AND CARNITINE METABOLISM.

Maxim V. Berezovski[1], Emil A. Zaripov[1], Abdullah Khraibah[1], Petr Kasyanchyk[1], Aliaksandra Radchanka[1], Nico Hüttmann[2], [1]Department of Chemistry and Biomolecular Sciences, University of Ottawa, ON K1N 6N5, Canada; [2]European Molecular Biology Laboratory, Molecular Systems Biology Unit, 69117, Germany. (maxim.berezovski@uottawa.ca)

A nano sheath-flow capillary electrophoresis mass spectrometry (CE-MS) system with electrospray ionization was used to profile cationic metabolite cargo in exosomes secreted by non-tumorigenic MCF-10A and tumorigenic MDA-MB-231 breast epithelial cells. An in-house produced sheath liquid interface was developed and machined from PEEK to enable nanoflow volumes. Normalization of CE-MS peak areas to total UV signal was employed to enhance quantitative accuracy and reduce variability. CE-MS-based metabolomics revealed increased purine synthesis intermediates and increased carnitine synthesis metabolites in MDA-MB-231-derived exosomes, with pathway enrichment indicating activation of de novo purine pathways and upregulation of carnitine metabolism. In addition, nanoLC-MS-based proteomics revealed differential expression of ecto-5'-nucleotidase (NT5E) and mitochondrial aldehyde dehydrogenase (ALDH9A1), demonstrating metabolic alterations in related enzymatic steps. This study demonstrates the application of nano sheath-flow CE-MS for comprehensive and quantitative exosome metabolomics, uncovering metabolic reprogramming in purine and carnitine pathways between normal and cancerous breast cell lines and providing insight into exosome-mediated signaling of breast cancer metabolism.

I030

AN AUTOMATED SYSTEM FOR THE ANALYSIS OF AS SPECIATION IN URINE AND HG SPECIATION IN BLOOD.

C. Derrick Quarles Jr.,[1] Nick Bohlim,[1] Patrick Sullivan,[1] Emily J Pacer,[2] Christopher Palmer,[2] Patrick J Parsons[2] . [1]Elemental Scientific, Inc., Omaha, NE, USA; [2]New York State Department of Health, Albany, NY, USA. (Derrick.Quarles@icpms.com)

Clinical laboratories are tasked with monitoring patient samples for exposure to harmful elements and reporting these values to healthcare officials. In the case for high levels of arsenic (As) or mercury (Hg), additional methods are required to determine the species so medical doctors can recommend the best course of action for the patient.

The work presented here will demonstrate a single platform system that is capable of inline sample preparation, chromatographic separation, and vapor generation in combination with ICPMS. Arsenic speciation in urine is carried out using a LC-ICPMS method, whereas Hg speciation in blood is carried out using a LC-ICPMS method with post-column vapor generation.

I031

DETERMINING THE PRIMARY REMOVAL MECHANISMS FOR ARSENIC IN LABORATORY-SCALE CONSTRUCTED WETLANDS BY COMBINING MASS BALANCE AND ARSENIC SPECIATION ANALYSIS FOR WASTEWATER, PLANTS AND BIOFILMS.

Antoine Hnain[1], Iris Koch[1], Debora Meira[2] and Kela Weber[1]. [1]Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 13 General Crerar Crescent, Kingston, ON K7K 7B4, Canada; [2]Argonne National Laboratory, 9700 S. Cass Avenue, Lemont, IL 60439, U.S.A. (antoine.hnain@rmc.ca)

Twelve lab-scale wetlands divided into 4x3 treatments (non-aerated planted and unplanted, aerated planted and unplanted) were used to study the speciation and removal of 1 mg/L of As(V) in synthetic domestic wastewater over a 33-week period. Mass balance calculations for the arsenic in the wetlands showed that biofilms from non-aerated wetlands contained more arsenic than biofilms from aerated mesocosms. The mass of arsenic found in plants from planted wetlands was negligible (<1%). Arsenic speciation in wastewaters for day 6 samples for weeks 1, 6 and 14 were examined through HPLC-ICP-MS analysis for all treatments and only non-aerated systems contained a higher proportion of methylated arsenic species likely due to microbial activity. Speciation of arsenic in flash frozen detached biofilms were examined through X-ray adsorption spectroscopy and revealed that only biofilms from non-aerated systems had As(III) and As(III)-S species, perhaps orpiment. Dried biofilm samples were examined through X-ray fluorescence and X-ray diffraction analysis and revealed a high iron content and the presence of pyrite in the biofilms from non-aerated systems, respectively. We believe that sulfate and iron reducing bacteria in the non-aerated systems may have formed the pyrite which was able to adsorb As(V) and enhance arsenic removal.

I032

MULTI-MODAL LASER SAMPLING WITH LIBS AND LA.

C Derrick Quarles Jr.,[1] Benjamin T. Manard,[2] Alex Zirakparvar,[2] Hunter Andrews,[2] Joe Petrus,[3] Lisa Balke[4], Uwe Karst[4]. [1]Elemental Scientific, Inc., Omaha, NE, USA; [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA; [3]Elemental Scientific Lasers, Bozeman, MT, USA; [4]University of Münster, Münster, Germany. (Derrick.Quarles@icpms.com)

The use of laser ablation-inductively coupled plasma mass spectrometry (LA-ICPMS) and laser-induced breakdown spectroscopy (LIBS) have become popular analytical techniques for bulk analysis, depth profiling, quantitative analysis, and elemental imaging. LA-ICPMS provides excellent trace element detection limits, whereas, LIBS offers elemental coverage (e.g., H, N, O, and F) that LA-ICPMS is unable to provide. By combining these two techniques, which are very complimentary to each other, the entire periodic table is accessible.

In this work, a 193 nm nanosecond excimer laser (imageGEO) is combined with a high-speed laser ablation cell and two LIBS detectors (multi-channel CMOS detector and an ICCD based detector). Example applications for geological, nuclear, pharmaceutical, and lithium ion batteries will be presented using various mass spectrometers (triple quadrupole ICPMS, time-of-flight ICPMS, multi collector-ICPMS, and a triple quadrupole MS).

I033

KNOW WHAT YOU VAPE: METAL ANALYSIS OF CANNABIS LIQUIDS. **Zuzana Gajdosechova**[1], Joshua Marleau-Gillette[1], Matthew Polivchuk[2], Ivana Kosarac[3], Guru Prasad Katuri[3], Dharani Das[3], Ashley Cabecinha[4], Andrew Waye[4]. [1] National Research Council Canada, Metrology, 1200 Montreal Rd., Ottawa, ON, K1A 0R6, Canada; [2] Natural Resource Canada, 601 Booth St., Ottawa, ON, K1A 0E8, Canada; [3] Tobacco Control Directorate, Health Canada, Ottawa, ON K1A 0K9, Canada; [4] Office of Cannabis Science and Surveillance, Strategic Policy Directorate, Controlled Substances and Cannabis Branch, Health Canada, 150 Tunney's Pasture Drive, Ottawa, ON, K1A 0K9, Canada. (Zuzana.Gajdosechova@nrc-cnrc.gc.ca)

Vaping cannabis liquids is a convenient consumption method but carries health risks. A key concern is the presence of metal particles in vape liquids, even in legal products. Measuring these particles is challenging due to their inhomogeneous distribution. This study analyzed total metals in five samples of six cannabis vape liquids. Results showed that metals from vaping device components, particularly Co, Ni, and Zn, contributed to variability within batches, while all studied metals varied significantly between products. Single-particle ICP-MS detected Al, Co, Cr, Ni, Sn, and Zn particles in the liquids. To assess potential consumer exposure to these metal particles, vape pens were artificially vaped, and the generated aerosol was analyzed. While particle counts were too low for quantification, all tested aerosols contained Co, Cr, Ni, Pb, Sn, and Zn. To determine the origin of these particles, emptied cartridges were analyzed using SEM-EDS. The elemental composition of the metal components of the cartridges correlated well with the detected particles, providing clear evidence that cannabis vape liquids are contaminated by the metal parts of the vaping devices. Cracks on an unused device's connector pin suggested further contamination risks during use.

I034 P

QUICK DETERMINATION OF RARE EARTH ELEMENTS IN POWDERED REFRACTORY MATERIALS USING ELECTROTHERMAL VAPORIZATION WITH DETECTION BY INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **Yangyang Wang**, Sophia Kienast and Diane Beauchemin. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (15yw103@queensu.ca)

The determination of rare earth elements (REEs) in refractory materials by inductively coupled plasma (ICP) spectrometry with nebulization requires dissolution of these samples, which is difficult. This work presents an optimized method using electrothermal vaporization (ETV) coupled to ICP optical emission spectrometry for the direct determination of REEs in refractory geological materials. The small sample mass required with ETV allows faster analysis with greater sensitivity than with nebulization by eliminating the dilution that is inherent to dissolution and introducing more sample in the plasma compared to nebulization. Point-by-point internal standardization with an argon emission line compensates for the visible sample loading effect on the plasma. External calibration using standard solutions provided accurate results for 15 REEs (Ce, Dy, Er, Eu, Gd, Ho, La, Lu, Nd, Pr, Sm, Tb, Tm, Y, and Yb). In contrast, only REEs with certified concentrations in the certified reference materials (CRMs) used for external calibration encompassing those in the sample could be determined with CRMs. Adding at least 30 µL of high-purity water to the graphite boat containing solid samples enhanced sensitivity by 61% on average.

I035

ANALYSIS OF RADIUM-226 IN ENVIRONMENTAL SAMPLES FROM URANIUM TAILING MANAGEMENT LAKES BY MASS SPECTROMETRY. **Laurie Martin**[1], Dominic Larivière[1], Raoul-Marie Couture[1], Richard Goulet[2], Nicolas Reynier[2]. [1]Chemistry Department, Laval University, [2]CanmetMINES; Natural Resources Canada (laurie1340@outlook.com)

In the city of Elliot Lake, once dubbed the "uranium capital of the world," several lakes were converted into disposal sites for uranium mining residues. However, in recent years, increased concentrations of radium-226 in these lakes have been reported but not explained. Understanding the geochemical processes influencing radium concentrations in these lakes is therefore crucial. To do so, sediments and porewater samples collected from two sites will be prepare and analyzed for radium-226.

As part of this project, efforts were made to develop reliable analytical methods to accurately quantify radium concentrations in various environmental components (sediment, water and porewater). To achieve this, different preconcentration and separation techniques using resins were developed, tailored to water and sediment samples. Subsequently, ICP-MS analysis was performed to rapidly, sensitively and efficiently quantify radium in the samples.

This project thus provides an integrated approach to evaluate and monitor radium levels in the lacustrine environment, thereby providing crucial data to better understand the geochemical processes affecting radium.

I036

CHARACTERIZATION OF EXTRACTABLES IN DENTAL BITE GUARD USING GC-TOFMS (Gas Chromatography – Time-Of-Flight Mass Spectrometry). **Stephan Laperriere[1]**, David E. Alonso[2] and Joe Binkley[2]. [1]LECO Instruments ULC, 2205 Dunwin Drive, Mississauga, ON, L5L 1X1, Canada; [2]LECO Corporation, 3000 Lakeview Avenue, Saint Joseph, Michigan, 49085, USA. (stephan_laperriere@leco.com)

Dental bite guards are increasingly prescribed by dentists to prevent teeth grinding during sleep. Analysis is necessary to assess the potential for harmful substances that could transfer to the consumer during use. Over-the-counter dental bite guards were evaluated for this case study with Gas Chromatography and Time-Of-Flight Mass Spectrometry (GC-TOFMS). The benefits for highly sensitive non-targeted analyses will be demonstrated for detection and characterization of both volatile and semi-volatile chemical constituents in the dental bite guard products. The volatile chemical constituents were characterized using headspace GC-TOFMS and the semi-volatile chemical constituents were characterized via liquid injection of the extracts obtained from the bite guards. Extractables that were above a calculated analytical evaluation threshold (AET) were characterized and identified in this study. Identifications were determined based on mass spectral library database matches (NIST 23 and Wiley 12) and supporting retention index (RI) determinations. Those that did not match commercial mass spectral libraries were further analyzed using GC with high resolution TOFMS, utilizing a multi-mode ionization source to acquire both electron and chemical ionization (EI & CI) spectra on the same source, to aid in structural elucidation. The chemical constituents determined in this characterization included residual monomers, polymer additives, and process impurities.

I037

ACCURATE SEX DETERMINATION OF MUMMIES THROUGH THE MULTI-ELEMENTAL ANALYSIS OF BONE TISSUE USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **Margaret MacConnachie[1]**, Jocelyn Williams[2], and Diane Beauchemin[3]. [1]Mount Royal University, Department of Chemistry and Physics, 4825 Mount Royal Gate SW, Calgary, AB T3E 6K6, Canada; [2]Trent University, Department of Anthropology, 1600 West Bank Drive, Peterborough, ON K9L 0G2, Canada; [3]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (mmacconnachie@mtroyal.ca)

Sex determination of human remains is vital within the field of archaeology, as it provides a more complete picture of social and biological structures that existed within ancient societies. Typically performed through examination of bones in the pelvic region, accurate sex determination can be exceedingly challenging in the absence of a sufficiently preserved skeleton. Here, a method for sex determination in mummies, involving measurement of magnesium, strontium, sulfur, and zinc in head hair along with multivariate statistics [1], was applied for the first time to bone tissue collected from 500-year-old mummies originating from Peru. The elemental markers for sex are present in bone tissue, highlighting their potential use for archaeologists, and indicating no significant diagenetic effects in the samples. Using the elemental information in the bone tissue, accurate sex predictions were achieved for all samples with a high degree of precision. Additionally, elemental content of the bone tissue was compared to that of hair samples from the same mummified individuals. This work lays the foundation for non-morphological sex determination methods within archaeology, filling a significant gap in the field.

[1] M. MacConnachie, S. Lu, Y. Wang, J. Williams, D. Beauchemin, RSC Adv. (2022) 27064-27071

I038

MULTIOMICS WORKFLOWS FOR BIOMARKER DISCOVERY IN DISEASE MODELS **Lekha Sleno**, Nathan Ghafari, Oriana Zambito, Maggy Lépine. Chemistry department/CERMO-FC, University of Quebec in Montreal (UQAM), Montreal, QC, Canada. (sleno.lekha@uqam.ca)

Our recent work on implementing developed untargeted and targeted metabolomics and proteomics will be presented. Metabolomics and proteomics provide complementary information for a better understanding of the mechanisms underlying specific pathological states by studying what biological pathways are dysregulated in model of diseases. We have developed a multiomics approach to study different mouse models of disease, including mucopolysaccharidosis type 2, polycystic ovarian syndrome, and Hirschsprung's disease. A combination of untargeted and targeted metabolomics as well as untargeted proteomics methods were used to observe metabolic variations in different sample types, including liver, colon, feces and plasma. In each case, we have identified several putative metabolites and proteins that are significantly different in the disease model compared to the control wild-type mouse. We also have investigated the effect of specific treatments of each of these diseases, and whether the metabolite or protein levels are reestablished to control levels or not. This approach can help find biomarkers of disease, decipher pathways that are perturbed as a consequence of the disease and examine if any of these biomarkers can be indicative of a positive treatment response. This presentation will discuss the advantages of combining different datasets in multi-omics workflows.

I039 P

SYNTHESIS AND CHARACTERIZATION OF 2,6-DI(THIAZOL-2-YL)ISONICOTINIC ACID AS A DUAL SENSOR FOR Fe^{2+} AND Hg^{2+}. **Yelyzaveta V. Antsybora**, Paola Canas, Cordelia Adams, Nisha R. Agarwal, Olena V. Zenkina. Ontario Tech University, Faculty of Science, 2000 Simcoe St N, Oshawa, ON L1G 0C5, Canada. (olena.zenkina@ontariotechu.ca)

Detection of mercury (Hg(2+)) is a key challenge facing modern society. Mercury is an extremely prevalent toxic metal ion occurring in various natural (volcanic eruptions, weathering of rocks) and anthropogenic sources (batteries, dental amalgam). Therefore, molecular receptors that are able to detect and differentiate mercury in solution are in high demand. Our previous study demonstrated 2,6-bis(2-thienyl)pyridine to be highly selective towards Hg(2+).[1] However, for these and many other receptors, the challenge is to overcome interference with more environmentally abundant transition metals (Fe(2+), Fe(3+), Zn(2+) etc.) Terpyridines are well-known chelators in analytical chemistry for their high affinity towards Fe(2+) and Fe(3+). In this study we present a modified dual purpose 2,6-di(thiazol-2-yl)pyridine core for simultaneous selective sensing of Fe(2+), Fe(3+), and Hg(2+). Structure of the probes containing the proposed core was comprehensively studied with 1D, 2D NMR techniques and mass spectroscopy. We demonstrated here that combination of fluorimetry and UV-Vis spectroscopy allow selective detection of abovementioned ions in the solution. Currently we are working on the expansion of initial finding towards the creation of solid state material series based on the 2,6-di(thiazol-2-yl)pyridine core.

[1] Egan, Hynes, Fruehwald, Ebralidze, King, Esfahani, Naumkin, Easton, Zenkina, J. Mater. Chem. C, 7 (2019) 10187 – 10195.

I040

MONOLAYERS OF TERPYRIDINE COMPLEXES FOR ULTRA-STABLE ELECTROCHROMIC DEVICES: DOUBLE-SIDE ARCHITECTURES. Marjan Saedi, Vittoria Di-Palo, E. Bradley Easton, **Olena V. Zenkina.** Ontario Tech. University, 2000 Simcoe Street North, Oshawa, Ontario, Canada. (Olena.zenkina@ontariotechu.ca)

In this work, we present methodologies for creating effective, novel double-sided symmetric and asymmetric architectures of solid-state electrochromic devices based on monolayers of *bis*-terpyridine iron and osmium metal complexes covalently embedded into suitable conductive metal oxide support.[1] Resulting novel, nonconventional double-side electrochromic devices demonstrate fast switching times, high coloration efficiencies, and colour contrasts and were able to withstand more than 100,000 consecutive electrochemical cycles. Separately, the role of the additional *Nafion* layer on the performance and stability of the devices was studied, and possible mechanisms of the device degradation were explored. The superior long-term durability of the double-sided architectures makes them very promising for future practical applications for the creation of smart double-sided signage, smart boards, non-emissive displays, and other smart interactive devices that change their colour upon application of a voltage.

[1] (a) DiPalo, V.-A.; Ahmad, R.; Ebralidze, I. I.; Mapue, N. D.; Easton, E. B.; Zenkina, O. V., *ACS Applied Materials & Interfaces* **2024,** *16* (1), 1082-1095; (b) DiPalo, V.-A.; Saeidi, M.; Ahmad, R.; Ebralidze, I. I.; Easton, E. B.; Zenkina, O. V., *Sol. Energy Mater. Sol. Cells* **2024,** *274*, 112963.

I041

FROM RELATIVE TO ABSOLUTE ELECTROCHEMILUMINESCENCE QUANTUM EFFICIENCIES OF METAL NANOCLUSTERS.

Kenneth Chu, Jonathan Adsetts, Xiaoli Qin, **Zhifeng Ding,** Department of Chemistry, Western University, 1151 Richmond Street, London, ON N6A5B7, Canada. (zfding@uwo.ca)

Our lab at Western focuses on 4 research themes: scanning electrochemical microscopy of live cells, ionic liquids as novel electrolytes, electrochemiluminescence (ECL) and solar cells. Herein, we summarize our ECL research on Au nanoclusters Au_{18}, Au_{25}, Au_{21}, Au_{25}, Au_{38} and Ag ones $PtAg_{28}$, $PtAg_{30}$. Correlation between nanocluster structures and their electrochemiluminescence (ECL) has been identified. We will show how crystal structures of Au and Ag nanoclusters determine their photoelectrochemical reactivity, revealed by means of ECL and photoluminescence spectroscopy. Photoelectrochemical reactivity as well as ECL mechanisms were elucidated based on electrochemistry, spooling photoluminescence, and spooling ECL spectroscopy. Three ECL enhancement origins in the nanocluster coreactant systems will be demonstrated: (i) effectively exposed reactive facets available to undergo electron transfer reactions; (ii) individual excited-state regeneration loops; (iii) cascade generations of various exited states. The determination of nanocluster absolute ECL quantum efficiencies will be demonstrated.

[1] M. Hesari, Z. Ding, *J. Am. Chem. Soc.*, **2021**, *143*, 19474-19485.
[2] Wei, X.; Chu, K.; Adsetts, J. R.; Li, H.; Kang, X.; Ding, Z.; Zhu, M., *J. Am. Chem. Soc.* **2022,** *144*, 20421-20433.
[3] Adsetts, J. R.; Chu, K.; Hesari, M.; Whitworth, Z.; Qin, X.; Zhan, Z.; Ding, Z., *J. Phys. Chem. C* **2022,** *126*, 20155–20162.

I042

TRACE ELEMENT SPECIATION ANALYSIS IN FOODSTUFFS – FROM RESEARCH TO REGULATION.

Jens J. Sloth, National Food Institute, Technical University of Denmark (DTU FOOD). (jjsl@food.dtu.dk)

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

Trace element speciation analysis has been among the most important research topics within the field of trace element analysis over the last decades. Food samples are comprised of a high variety of chemical compounds from which many can interact with the elements and form (complex) elemental species with relevance to food quality/safety evaluation. In order to achieve the full picture it is important not only to determine the total amount of a certain trace element present in the food sample but also to identify the chemical form in which given element occurs in given sample (i.e. its speciation). Selected examples on trace element speciation will be presented with a focus on development and application of methods aiming at control of food safety aspects.
Selected examples from research activities on speciation will be presented and how speciation analysis is also now being part of official food control.

I043

ELEMENTAL SPECIATION AT THE FDA'S NATIONAL FORENSIC CHEMISTY CENTER

Kevin Kubachka, Nicole Walker, Bedraj Pandey, and Rachel Dicken, US FDA's National Forensic Chemistry Center, 6751 Steger Drive, Cincinnati, OH 45237, U.S.A. (kevin.kubachka@fda.hhs.gov)

Elemental analysis of FDA regulated products is an important area of interest to public health. The chemical species of an element strongly affects toxicity, health benefit, absorption, etc. The total elemental concentration in a sample often does not provide adequate information for risk or benefit analysis. The US FDA's National Forensic Chemistry Center (NFCC) has utilized elemental speciation for a variety of applications, including contaminant detection and label verification in foods, drugs, and dietary supplements. Elements encountered in our laboratory requiring accurate, robust, validated speciation methods include arsenic, selenium, chromium, iodine, mercury, and silver.

Due to the range of contaminants and ingredients of interest, in a wide variety of matrices, specialized treatment for sample preparation, interferences, and speciation is required. This presentation will focus on applications of elemental speciation to solve problems encountered by the NFCC and other FDA laboratories. Additionally, current progress of related research projects (including the synthesis of a newly identified arsenical present in rice) and on-going method validations will be discussed.

I044

FORMATION OF ARSENOBETAINE. **Iris Koch[1]**, Blaire Coffey[1], Jennifer Scott[2], [1]Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 12 Verité Ave, 17000 Station Forces, Kingston, ON K7K 7B4, Canada; [2]Laurentian University, Sudbury, Ontario, Canada. (koch-i@rmc.ca)

Arsenic is well-known as a poison but the chemical form determines the toxicity of arsenic compounds. Only one arsenical, arsenobetaine, is largely considered to be non-toxic; it is found as the predominant arsenical in marine fish and some terrestrial fungi, which have higher natural arsenic concentrations than most other biological media, and are important as food for human consumption. We have specifically been studying the abiotic formation of arsenobetaine from trimethylarsine oxide, haloacetic acids, and glutathione. Chloro-, bromo-, and iodoacetic acids all promoted the formation of arsenobetaine in the reaction pathway to the same extent. We found chloroacetic acid in Ontario rainwater, helping to support the plausibility of the reaction taking place in the environment. No arsenobetaine was formed in any reactions that did not include glutathione, including oxygen-free reactions with soil associated with arsenobetaine-containing mushrooms. As it is probable that the trimethylarsine oxide must be reduced for the reaction to proceed, any reducing agents occurring in the soil appeared to be insufficient in our experimental conditions for the reducing step, and we continue to investigate the need and efficacy of biologically-derived reducing agents.

I045

PRELIMINARY RISK ASSESSMENT OF GARDEN VEGETABLES IN YELLOWKNIFE, NORTHWEST TERRITORIES. **Iris Koch[1]**, Andre Castillo[2], Diane Beauchemin[2], Mike Palmer[3], [1]Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 12 Verité Ave, 17000 Station Forces, Kingston, ON K7K 7B4, Canada; [2]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; [3]North Slave Research Centre, Aurora Research Institute, Aurora College, Yellowknife, NWT X1A 2R3, Canada. (koch-i@rmc.ca)

The Yellowknife Garden Metal Study (YKGMS) was initiated to address concerns about the impact of legacy mining in the area in light of the increase of agricultural initiatives in Yellowknife and increasing popularity of growing vegetables for personal consumption. The study was designed to quantify and understand the impacts of potentially harmful elements resulting from the historical mining activities. Preliminary results of a human health risk assessment (HHRA) conducted on the first year of vegetable data were presented in 2021 to the community and stakeholders, and the process of the HHRA, results, and communication strategy will be described in the presentation.

I046

GRAFTING VERSATILE MONOLITHIC SUPPORTS IN MICROCHANNELS FOR THE SCREENING OF DECORPORATION MOLECULES AND THE SOLID PHASE EXTRACTION OF RADIONUCLIDES. **N. Ivanov**[1], S. Mekkaoui[1], M. Monnin[1], M. Boudias[1], A. Van der Meeren[2], O. Grémy[2], C. Bresson[1]. [1] Université Paris-Saclay, CEA, Service de Physico-Chimie, 91191 Gif-sur-Yvette, France; [2] Laboratoire de Radiotoxicologie, CEA, Université Paris-Saclay, 91297 Arpajon, France. (nikita.ivanov@cea.fr)

The downscaling of analytical procedures typically performed in laboratories leads to decreasing material consumption and waste generation, which is especially crucial in the nuclear sector. In this regard, we concentrate on the miniaturization of purification and separation steps of samples that contain radionuclides (RNs). A highly effective strategy for addressing miniaturization is to synthesize *in-situ* monolithic polymers in micro-channels. Monoliths exhibit high specific surface area, adjustable morphology and are highly versatile, since they can be functionalized to meet various objectives, ranging from sample purification by solid phase extraction, to complex analysis where RN-loaded monoliths are used to screen RNs decorporation agents. In line with this reasoning, the goal of this project is to develop a miniaturized, multiplex device to assess the affinity and selectivity of candidate molecules for uranium (U), cesium (Cs), strontium (Sr), or cobalt (Co) decorporation. The coupling of the microsystem to ICP-MS and ESI-MS allows to assess the RN-loading capacity of each monolith alongside the chelating power of the eluted molecules based on their affinity for the immobilized RNs. The most promising chelator-RN couples will be subject to additional *ex-vivo* and *in-vitro* tests in physiological conditions.

I047

EXPLORING DIGESTION METHODS FOR INSOLUBLE MANGANESE (MN) IN PREPARATION FOR ELECTROCHEMICAL DETECTION IN DRINKING WATER. **Kayla Elliott**, Zhe She, and Sarah Jane Payne, Queen's University, Department of Chemistry and Department of Civil Engineering, Kingston, ON, Canada. (19kle2@queensu.ca)

Manganese (Mn) is a contaminant of emerging concern present in drinking water that has shown to have negative neurological effects on children. In drinking water, Mn exists as soluble Mn (II) and insoluble Mn (IV), and is regulated based on total Mn levels, including both soluble and insoluble species. While there exist effective treatment processes to remove Mn, trace levels leaving the treatment plant may accumulate in the distribution system as reservoirs that can be rereleased into the bulk water at dangerous concentration levels. Traditional spectroscopic techniques for Mn monitoring are not practicable for on-site detection due to their size and cost. Alternatively, electrochemical methods, which are promising for on-site monitoring are limited to the measurement of dissolved species. Therefore, there is critical need for the development of an electrochemical method that offers the advantage of on-site monitoring and can detect total Mn content in drinking water. This work explores digestion procedures to prepare samples containing insoluble Mn for electrochemical detection. Parameters including pH, digestion time, Mn concentration and the presence of common interferents are considered. This research will allow for all forms of Mn, including insoluble species to be monitored on-site and represent a breakthrough in Mn management technology.

I048

A RAPID METHOD FOR ARSENIC SPECIATION IN URINE AND FOOD MATRICES USING ISOCRATIC ELUTION LC-ICP-MS/MS. Austin A. Roberts, Christopher D. Palmer and **Patrick J. Parsons**. Division of Environmental Health Sciences, Wadsworth Center, NY State Department of Health, Albany, NY 12237, USA; and Department of Environmental Health Sciences, University at Albany, Rensselaer, NY 12114, USA.(patrick.parsons@health.ny.gov)

A simplified method for As speciation in urine was developed for human biomonitoring studies. Ion-pairing LC on a 25-cm C18 column is used with isocratic elution to avoid long re-equilibration times between samples. Urine is treated with H_2O_2 to oxidize As^{3+} to As^{5+} thus avoiding the need to 'flash freeze' urine samples immediately after collection to prevent interconversion. The combined As^{3+} + As^{5+} is reported as "inorganic As" (iAs). Five species are measured including arsenocholine, arsenobetaine, dimethylarsinic acid, monomethylarsonic acid, and iAs, with method LODs (3σ) = 0.19, 0.19, 0.53, 0.34, 0.46 µg/L respectively. An internal standard (As^{5+}) is injected post-column *via* a 6-port switching valve with detection by ICP-MS/MS at m/z 91 in O_2 gas mode. The method was validated against NIST SRM 2669 Arsenic Species in Frozen Human Urine. Satisfactory performance in three proficiency testing schemes (CDC PAsS, GEQUAS, and CTQ) was demonstrated. The method was extended to food matrices by incorporating a 2-hour microwave-assisted extraction step with 50:50 MeOH:H_2O at 90 °C. Extracts are filtered and As species separated using the same LC method. Method validation for food matrices included NIST SRM 1568b, NRC DORM 4 and NRC TORT 3, with LODs ranging from 9 –11 ng/g.

I049

SENSITIVITY-ENHANCED SOLID-STATE NMR SPECTROSCOPY OF HETEROGENEOUS MATERIALS.

Lucas Urbano José[1], Rishi Verma,[2] Ankit Dhakal,[3] Gaurav Giri,[3] Ulla Gro Nielsen,[1,4] Vivek Polshettiwar,[2] **Amrit Venkatesh**[5]. [1]Department of Physics, Chemistry, and Pharmacy, University of Southern Denmark, 5230 Odense M, Denmark; [2]Department of Chemical Sciences, Tata Institute of Fundamental Research (TIFR), India; [3]Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22904, USA; [4]Novo Nordisk Fonden, Tuborg Havnevej 19, 2900 Hellerup, Denmark; [5]Department of Chemistry, University of Virginia, Charlottesville, VA 22904, USA. (amrit.venkatesh@virginia.edu)

The rational design of materials and determination of structure-property relationships requires a detailed analytical characterization. Solid-state NMR spectroscopy enhanced by high magnetic fields, fast magic angle spinning and dynamic nuclear polarization is a powerful way to interrogate local environments of nuclei across the periodic table that may be present in materials, and correlate structure to function. Here we show how sensitivity-enhanced multinuclear solid-state NMR spectroscopy can provide an atomic-level understanding on heterogeneous materials. The local structure environments in defected amorphous aluminosilicates that are used as catalytic support materials will be described. Next, the effect of phosphate uptake on MgAl layered double hydroxides and the identification of phosphate binding sites will be discussed. Finally, the structure of UiO66/P(VDF-TrFE) metal organic framework – polymer composites synthesized by in-situ crystallization for application as piezoelectrics will be described. These examples demonstrate the versatility of solid-state NMR spectroscopy in the materials chemistry toolkit.

I050

ENVIRONMENTAL APPLICATIONS OF SPECIATION ANALYSIS.

Ben Wozniak, Brooks Applied Labs, LLC, 13751 Lake City Way NE, Seattle, WA 98125, USA. (ben@brooksapplied.com)

Different chemical species or molecular forms of an element exhibit varying properties, which influence their fate, transport, bioavailability, and effects in the environment. For example, arsenate is typically less mobile in groundwater than arsenite due to its stronger sorption to soils; methylated selenium species may have a greater impact than inorganic selenium in aquatic environments because they are more readily absorbed by organisms; and trivalent chromium is an essential nutrient whereas hexavalent chromium is a known carcinogen. While determining the total concentration of an element in an environmental compartment (*e.g.*, water, soil, air, or biota) is crucial for understanding its distribution and behaviour, measuring discrete chemical species is often necessary for evaluating potential effects. When significant environmental contamination is detected, speciation data can also provide valuable insights that improve the efficiency and efficacy of remediation efforts.

Drawing on Brooks Applied Labs' decades of experience performing such analyses, environmental applications highlighting the importance of speciation will be presented for multiple elements. Emphases will be placed on less commonly considered species (*e.g.*, thioarsenicals), potential procedural pitfalls, and quality assurance considerations.

I051

MAPPING OXYLIPIN DEGRADATION PATHWAYS USING LC-HRMS Oluwatosin Kuteyi, **Dajana Vuckovic**, Concordia University, 7141 Sherbrooke Street West, Montréal, QC, Canada. (dajana.vuckovic@concordia.ca)

Oxylipins are lipid mediators involved in inflammation, immunity, and oxidative stress. Accurately measuring oxylipins in biospecimens is analytically challenging due to their poor stability and susceptibility to both enzymatic and non-enzymatic reactions during sampling, storage, and transportation. Recently, in vivo solid-phase microextraction (SPME) has been introduced as an effective method for direct sampling and extraction of oxylipins from biological tissues and fluids. In this study, we first investigated how the storage of oxylipins on the SPME devices affects oxylipin stability and susceptibility to non-enzymatic reactions such as autoxidation, hydrolysis, and isomerization. We next showed that antioxidant such as butylated hydroxytoluene (BHT) was not broadly useful to minimize auto-oxidation. Lastly, unstable oxylipins were subjected to forced degradation studies including photooxidation (365 nm for 5 and 7 days), copper sulphate oxidation, and elevated temperatures (37°C and 50°C for 3 days) to map their degradation pathways using LC-HRMS. This study provides important insights into major degradation products of PUFAs and selected oxylipins. Importantly, these results also show how the degradation of unstable oxylipins can impact the accurate measurement of stable oxylipins, thus representing an under-appreciated source of error during the measurement.

I052 (2024 Award presentation)

LIPIDOMICS ODYSSEY: CURRENT STATUS AND FUTURE HORIZONS. Lise Cougnaud, Reza Maulana, Ana Carolina Dos Santos, Elissa Mariani, **Dajana Vuckovic**, Concordia University, 7141 Sherbrooke Street West, Montréal, Canada. (dajana.vuckovic@concordia.ca)

Liquid chromatography – mass spectrometry is currently the most powerful technique for metabolomics and lipidomics due to unprecedented molecular coverage provided by fast and highly sensitive modern mass spectrometers. However, high-quality large-scale lipidomics data sets are urgently needed, in order to provide more systematic understanding of lipid dynamics and successfully validate and translate new biomarkers into the clinic. Analytical chemistry and separation science have a critical role to play in this journey to truly harness the power of metabolomics/lipidomics. In this talk, I will discuss several challenges and advances in lipidomics of biological fluids and tissue. These include (i) sample integrity and ensuring the measured lipidome is reflective of the true lipidome at the time of sampling, (ii) measuring low abundance lipids and expanding coverage of lipidomics methods, (iii) moving towards microsampling and real-time at-home sample collection and (iv) increasing quality control and data quality. Specifically, I will focus on how in vivo solid-phase microextraction can be used for longitudinal sampling of tissues and/or biofluids including challenging analytes such as oxylipins. Finally, I will highlight key results from recent inter-laboratory studies and discuss how adduct formation and internal standard selection play critical role in accuracy and data harmonization across studies.

I053

DESTRUCTION AND TRANSFORMATION OF PFAS IN CONTAMINATED SOIL VIA BALL MILLING: ANALYSIS CONSIDERATIONS AND CURRENT PROGRESS.

D. Morrow, N. Battye, T. Brown, A. Pang, I. Koch, **K.P. Weber**, Environmental Sciences Group – Royal Military College of Canada, Kingston, ON, Canada. (kela.weber@rmc.ca)

Per- and polyfluoroalkyl substances (PFAS) are chemicals which contain one or more carbon atom and one or more fluorine atom. Over the last 60 years at least 4000 different PFAS have been incorporated into industrial and commercial products and subsequently released to the environment. Many PFAS are understood to bioaccumulate and have toxicological properties. Regulatory guidance is currently challenged due to a lack of economically viable PFAS remediation and/or management options. The carbon-fluorine bond(s) make PFAS resistant to degradation. Many PFAS have however been shown to readily transform both in the lab and the field under varying conditions. Transformation of PFAS has also been seen in the development and employment of many remediation technologies. This however is not desired as the transformation products could have greater toxicities than the original parent PFAS. This talk will describe several projects involving the destruction and transformation of PFAS in soil via mechanochemical action (ball milling). Mechanistic insights, analytical challenges and considerations, and the potential paths forward will be discussed.

I054

UNRAVELING CO2 CHEMISORPTION MECHANISMS IN CYCLODEXTRIN-BASED MOFS: INSIGHTS FROM SOLID-STATE NMR SPECTROSCOPY.

Tahereh Azizivahed and Yining Huang. The University of Western Ontario, Department of Chemistry, 1151 Richmond Street, London, N6A 5B7, Canada. (taziziva@uwo.ca, yhuang@uwo.ca)

Global warming, driven by rising greenhouse gases like CO2, leads to climate change and a cascade of other environmental impacts. Consequently, there is growing demand for efficient CO2 adsorption methods to capture emissions before they enter the carbon cycle or extract them directly from the atmosphere. Porous materials, especially Metal-Organic Frameworks (MOFs), have shown remarkable potential in this area. Among these materials, Cyclodextrin-based MOFs (CDMOFs), as sustainable and biocompatible molecular sieves, stand out due to their excellent ability to selectively chemisorb CO2. This exceptional property can be attributed to the presence of nucleophilic hydroxyl sites within the framework. The hydroxide nucleophiles can reversibly react with CO2 to form (bi)carbonate species;1 however, the exact mechanism governing this reaction is not yet fully understood and requires further investigation. In this work, we harness multinuclear and multidimensional SSNMR spectroscopy to elucidate the interactions between CO2 and hydroxyl groups on both the primary and secondary faces of CD-MOFs, including chargebalancing OH- sites, by probing nuclei such as 13C, 17O, 1H, 87Rb, and 39K, thereby clarifying the chemisorption mechanism and the role of water molecules.

[1] (2022). Zick, M. E., Pugh, S. M., Lee, J.-H., Forse, A. C. & Milner, P. J. Angewandte Chemie 134,

I055

ELECTROCHEMILUMINESCENCE AND PHOTOLUMINESCENCE OF GRAPHENE QUANTUM DOTS **Zhenzhong Cai**, Congyang Zhang and Zhifeng Ding Department of Chemistry, Western University, 1151 Richmond Steet, London, ON N6A 5B7, Canada. (zcai66@uwo.ca)

Graphene quantum dots (GQDs) have emerged as promising nanomaterials in analytical and spectroscopic applications due to their tunable optical properties. In this study, we synthesized GQDs via electrochemical exfoliation at varying current densities and investigated their electrochemiluminescence (ECL) behaviors and mechanisms using electrochemical and spectroscopic techniques. Photoluminescence and UV–visible absorption spectroscopy revealed surface-state contributions to long-wavelength emission, while spooling ECL spectroscopy demonstrated the influence of exciplex formation in aggregation-induced emission. Cyclic voltammetry coupled with ECL-voltage curves confirmed the presence of surface-trapped excitons and charge-transfer interactions. The absolute ECL quantum efficiency of GQDs reached as high as (0.028 ± 0.002%), demonstrating their efficiency in electron-to-photon conversion. These findings provide deeper insights into the structure-property relationships governing GQD-based ECL, advancing their potential for analytical sensing, bioimaging, and optoelectronic applications.

[1] Zhang, C.; Cai, Z.; Chu, K.; Shiu, W.-T.; Hu, P.; Liu, L.; Zhang, Q.; Ding, Z., Exploring Surface State and Exciplex Dominated Aggregation Induced Electrochemiluminescence of Graphene Quantum Dots Prepared Via Electrochemical Exfoliation. ChemPhysChem 2025, e202401074.

I056

REMEDIATION OF PFAS CONTAMINATION IN GROUNDWATER BY UV ACTIVATED SULFITE/IODIDE SYSTEM. Iris Koch, Adrian Pang, Kela Weber, **Yang Xu**, Royal Military College of Canada, Environmental Sciences Group, 12 Verite Ave, Kingston, ON K7K 5P2, Canada. (Yang.Xu@rmc-cmr.ca)

Per and polyfluoroalkyl substances (PFAS) are a large class of synthetic organofluorine compounds which demonstrate many desirable properties such as hydrophobicity, oleophobicity, tensioactivity, and exceptional stability. These properties have led to their widespread use in industry and commercial applications, and subsequently their ubiquity in the environment. Concerns surrounding environmental contamination of PFAS have mounted with increasing evidence of the toxicological effects of many of these PFAS compounds. While absorptive and filtration technologies are successful at removing PFAS from the environment, the development of an effective destructive technology is required to address the issue of PFAS contamination. UV/Sulfite/Iodide systems have achieved complete degradation of notoriously recalcitrant PFAS compounds in water at a laboratory scale. However, successful implementation of this technology in real-world applications requires further development to meet the challenges posed by more complex environmental matrices such as groundwater. This study aims to assess the feasibility of UV/Sulfite/Iodide systems in the treatment of groundwater by identifying the effects of various groundwater constituents.

I057

CHARACTERIZATION AND ANALYSIS OF MINERAL DEPOSITS DISCOVERED IN AIRCRAFT RESCUE AND FIREFIGHTING VEHICLES (ARFFV).

Adrian Pang[1], Chris Kocur[1], Taylor Vereecken[1], Ryan Mason[2], Stefanie Goure[3], Rick Dunning[4], Dana Pantea[4], Iris Koch[1] and Kela Weber[1]. [1]Environmental Sciences Group, Royal Military College of Canada 13 Crerar Crescent, PO Box 17000, Station Forces, Kingston, ON, Canada; [2]St. Lawrence College, 100 Portsmouth Ave, Kingston, ON, Canada; [3]Director Land Environment, Canadian Army, 45 Sacré-coeur Blvd Gatineau, QB, Canada; [4]Department Of National Defence, Government of Canada, 3500 Carling Avenue, Ottawa, ON, Canada. (adrian.pang2@rmc-cmr.ca)

Aqueous firefighting foams (AFFF) contain high amounts of per- and polyfluoroalkyl substances (PFAS), a large class of anthropogenic organofluorine compounds. As more toxicological data regarding the exposure of PFAS is discovered, governments are initiating the transition away from the use of AFFF to fluorine-free foams. To mitigate the discharge of residual PFAS due to cross-contamination, there exists the need to decontaminate the PFAS-impacted storage tanks of ARFFVs. Previous attempts at decontaminating ARFFVs to below regulatory guideline values have been unsuccessful. This may be due to the presence of mineral deposits sometimes found within the ARFFVs that do not dissolve readily and cannot be flushed out easily. This study aims to characterize mineral deposits found within an ARFFV tank and to determine extent of PFAS adsorption within these deposits. Mineral deposits were characterized using powder X-ray diffraction (PXRD), Brunauer–Emmett–Teller (BET), energy dispersive X-ray spectroscopy (EDX) and thermal gravimetric analysis (TGA). The materials were also subjected to washing and subsequently soaked in solvents to estimate the amount of PFAS adsorbed with the crystalline structure.

I058

SELECTIVITY OF ARSENOBETAINE USING FIELD PORTABLE X-RAY FLUORESCENCE.

Blaire Coffey, Jennifer Scott, and Iris Koch. Royal Military College of Canada, Department of Chemistry and Chemical Engineering, Environmental Sciences Group, PO Box 17000, Station Forces, Kingston, ON K7K 7B4, Canada. (blaire.coffey@rmc.ca)

Arsenic is a widely distributed element within the environment. This metalloid can be found in a variety of chemical forms. Arsenic is commonly known as a poison and carcinogen; however, arsenic compounds display different toxicities. Generally, inorganic arsenic forms, including arsenite and arsenate, are more toxic. Organoarsenic compounds, specifically those in the pentavalent form, are less toxic. One organoarsenic compound, arsenobetaine (AB), exhibits non-toxic properties. AB is predominantly found in marine organisms and less commonly found in the terrestrial environment with the exception of fruiting bodies (or mushrooms) of some terrestrial fungi species. Currently, AB's role and formation in mushrooms is unknown. It is hypothesized that AB acts as an osmolyte within the mushroom. This presentation examines potential abiotic formation pathways for AB. One proposed pathway involves exposing trimethylarsine oxide to a haloacetic acid in the presence of glutathione. To investigate this pathway, various synthetic reactions were conducted. These reactions were analyzed for arsenic speciation using HPLC-ICP-MS targeting AB. Additionally, a field portable x-ray fluorescence based method was developed to provide real-time analysis of AB in solid and liquid samples. This method was verified using synchrotron-based x-ray absorption near edge structure analysis at the Advanced Photon Source in Chicago, IL.

I059

INVESTIGATION OF ARSENIC SPECIES IN CANADIAN PEATBOGS.

Helen Lord,[1] Andrea Raab,[2] Joerg Feldmann,[2] Iris Koch,[3] and Diane Beauchemin.[1] [1]Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada; [2]Karl-Franzens University of Graz, 8010 Graz, Austria; Royal Military College of Canada, Kingston, ON, Canada. (17hgl1@queensu.ca)

The impact of peatlands on the biogeochemical cycling of As needs to be better understood because peatlands have the potential to be "hotspots for organoarsenical formation" [1]. In the environment, As from natural and anthropogenic sources can take different chemical forms having different toxicities. Arsenobetaine (AsB) is the only known stable, non-toxic and biologically safe As species, which is dominant in marine animals [2] and is generally less abundant in the terrestrial environment. However, AsB was found to be prevalent in peatlands in the United Kingdom [1]. The generally anoxic, waterlogged and organic conditions of peatlands may give this type of ecosystem the ability to form AsB [1]. The proposed mechanisms for the formation of AsB in the environment [2] are not definitive, and thus its source, especially in a terrestrial environment, is unknown. Most peatlands in Canada are in the North, but an urban parkland peatland in London Ontario, Sifton Bog, is a floating acid peat bog and an environmentally significant area. Preliminary and post sampling in Sifton Bog in 2022 and 2023 revealed As concentrations up to 30 mg/kg, which exceed provincial and federal soil quality guidelines. These results prompted the investigation of As species to determine if AsB could also exist in Canadian peatbogs. Using high performance liquid chromatography coupled to inductively coupled plasma mass spectrometry, AsB, and other As species, are detected in Sifton Bog.

[1] C. Mikutta, J.J. Rothwell, *Environ. Sci. Technol.* **2016**, *50* (8), 4314–4323.
[2] A. Popowich, Q. Zhang, X.C. Le, *National Science Review* **2016**, *3* (4), 451–458.

I060

THE INNOVATIVE AGILENT MICROWAVE PLASMA ATOMIC EMISSION SPECTROSCOPY AND WHERE TO USE IT.

Longbo Yang. Agilent Technologies, 6705 Millcreek Drive, Mississauga, ON L5N 8B3, Canada. (longbo.yang@agilent.com)

The Agilent Microwave Plasma–Atomic Emission Spectrometer (MP-AES) is a next-generation instrument for elemental analysis that combines performance, safety, and cost-efficiency. Different from traditional atomic technologies like Flame AA and ICP-OES, MP-AES utilizes nitrogen-based microwave plasma to excite atoms, removing the necessity for flammable gases like acetylene, and thereby improving laboratory safety and allowing unattended operation. By eliminating the need for costly gas cylinders, it offers the lowest cost of ownership among all atomic spectroscopy instruments while delivering high sensitivity and low detection limits across a wide range of elements. Free from the constraints of gas delivery, MP-AES can be deployed in remote locations including environmental monitoring stations and remote mine sites. With its combination of sensitivity, reliability and user-friendly operation, MP-AES is increasingly being adopted into routine elemental analysis in various applications such as environmental monitoring, agriculture, food safety, mining and material science.

I061

A NOVEL SUPERVISED LEARNING ALGORITHM FOR REAL-TIME COLLISION ENERGY SELECTION TO OPTIMIZE PEPTIDE FRAGMENTATION IN MASS SPECTROMETRY.

Yun-En Chung, University of Ottawa, Department of Biochemistry, Microbiology and Immunology, 451 Smyth Road, Ottawa, ON, K1H 8M5, Canada. Matthew Willetts, Bruker Daltonics Inc. Jens Decker, Bruker Daltonics Inc. Nagarjuna Nagaraj, Bruker Daltonics Inc., Jonathan R. Krieger, Bruker Ltd., Tharan Srikumar Bruker Ltd., **Mathieu Lavallée-Adam**, University of Ottawa, Department of Biochemistry, Microbiology and Immunology, 451 Smyth Road, Ottawa, ON K1H 8M5, Canada. (mathieu.lavallee@uottawa.ca)

The ability to identify peptides using mass spectrometry is directly linked to the fragmentation quality of peptide precursor ions. Precursor ion properties, such as mass-to-charge ratio (m/z) and charge state influence the level of collision energy required for optimal fragmentation of a given peptide. Nevertheless, most mass spectrometers do not make use of all these pieces of information when attempting to determine the optimal collision energy for an ion. Herein, we present a novel supervised learning strategy that uses precursor ion properties from mass spectrometry such as m/z, charge state and ion mobility coefficient to determine in real-time the collision energy level that optimizes precursor ion fragmentation. We show on a Bruker timsTOF Pro mass spectrometer operating in data-dependent acquisition that when our tool selects the optimal collision energy level for a given precursor ion, peptide and protein identifications from PEAKS de novo sequencing increase by 15% and 5%, respectively, compared to the instrument's default collision energy settings (false discovery rate (FDR)<1%). We also show that when applied to human cell lysates enriched for phosphorylated peptides, our method identified 10% more post-translationally modified peptides (FDR<1%). Overall, our novel precursor ion fragmentation optimization method improves peptide and post-translational modification identifications.

I062

ELECTROCHEMICAL CONVERSION OF SUBSTITUTED PHENOLIC DERIVATIVES.

Tyra Lewis, Sanela Martic, Trent University, Forensic Science, Environmental and Life Sciences, Materials Science, 1600 West Bank Dr., Peterborough, ON Canada. (sanelamartic@trentu.ca)

Phenolic compounds are of relevance to biotechnology, agriculture, and industry and may redistribute into the environment. The transformation of phenolic pollutants may be achieved by harsh chemical treatments. However, the selective transformation of phenolics into new functional molecules can also be achieved through milder, greener and more sustainable avenues like electrosynthesis [1]. Electro-oxidation of a phenol may generate a variety of products, including quinones, polymers and new carbon-carbon bond formation, resulting in new value-added chemicals of industrial interest. Herein, the electrochemical conversion of 2,6di-tert-butylphenol (DTBP), 2,6-diphenylphenol (DPP), and 5-chloro-2-(2,4dichlorophenoxy)phenol (triclosan) were compared to a traditional chemical oxidation process [2,3]. All compounds underwent oxidation following cyclic voltammetry or by addition of an oxidizing agent resulting in significant colour changes. The product formation was monitored by spectroscopy and characterized by X-ray single crystal diffraction and gas chromatographymass spectrometry (GC-MS). The electrochemical oxidation resulted in various products, including carbon-carbon bond formation with extended conjugation. Overall, the data suggest that the yield and selectivity of electrosynthesis are dependent on parameters used, and electrosynthesis may allow for reaction selectivity which is not achievable by chemical means.

[1] C.D. Cook, R.C. Woodworth, *J. Am. Chem. Soc*. 75 (1953) 6242-6244.
[2] N.L. Zabik, C.N. Virca, T.M. McCormick, S. Martic-Milne *J. Phys. Chem. B*. 120 (2016) 8914-8924.
[3] Lewis T., C.N. Gao S., D. Haas, S. Martic. *Electrocatal*. 15 (2024) 474-484.

I063

A DIGITAL SHADOW OF FRONT-END SEPARATION PERFORMANCE IN LC-MS/MS: METHODS FOR UNSUPERVISED ANALYSIS OF PUMP PRESSURE PROFILE CHANGES THAT PREDICT MICROFLUIDIC FAILURES. **Miroslava Cuperlovic-Culf**[1,2] Thao Nguyen-Tran[2-4], Roy Wang[5], Caitlin Fowler[1-3], Adam Mahdi[1,2], Irina Alecu[2,3], Ting Hu[5], Steffany A.L. Bennett[2-4]. [1]Digital Technologies Research Centre, National Research Council of Canada, 1200 Montreal Road, Ottawa, ON, Canada; [2]Department of Biochemistry, Microbiology, and Immunology, [3]Neurolipidomics Laboratory, Ottawa Institute of Systems Biology, Brain and Mind Research Institute, and [4]Department of Chemistry and Biomolecular Sciences, Centre for Catalysis Research and Innovation, University of Ottawa, Ottawa, ON, Canada; [5]Department of Computer Science, Queens University, Kingston, ON, Canada. (cuperlovim@nrc.ca)

Microfluidic problems in high performance liquid chromatography (LC) ultimately manifest as deviations from the expected pressure profile. The ability to predict emerging LC problems from acquisition pressure profiles would enable users to prevent LC-tandem mass spectrometry (MS/MS) failures, reduce costs, eliminate downtime, and accelerate research and output. To address this need, we present here an open-source cross-platform digital LC shadow that mirrors the operational state of front-end chromatographic separation systems and computationally alerts users to potential degradations in future performance. We present a combination of novel analysis strategies that automatically detects change points, both as a deviation from the trend and as an anomaly in performance, that vary from optimal performance reference values. Our digital LC shadow methodology combines different distance measures with unsupervised and supervised machine learning to characterize instrument acquisition performance and predict trends. We show computationally generated examples of different types and levels of change in LC-MS/MS pressure profiles, evaluating sensitivity and specificity of this novel methodology in comparison to real-world annotations of system maintenance. Although our digital LC shadow was built using data generated on an Agilent Infinity II High-Speed Binary Pump System coupled to a SCIEX QTRAP 5500 triple quadrupole linear ion trap mass spectrometer, it accepts input from any LC-MS/MS system that can output pump pressure profiles in real-time or at end of acquisition. The method can further be applied as a digital shadow for any longitudinal sensor tracking measure of performance problems in which failure ultimately manifests as deviations from expected values.

I064

NANOSTRUCTURED PLASMONIC SENSORS FOR THE DETECTION OF HAZARDOUS ANALYTES. **Carlos Escobedo**. Department of Chemical Engineering, Queen’s University, Kingston, ON, Canada. (ce32@queensu.ca)

Metallic nanostructures enable plasmon resonances that have encouraged their use as sensors. The localized surface plasmon resonance that metallic nanostructures produce is particularly effective in sensing spectroscopic applications, such as Raman. Surface-enhanced Raman scattering is a powerful technique that provide with highly resolved vibrational information of chemicals and biological specimens, with exceptional sensitivity. SERS-based detection schemes have become more amenable to be interfaced with optics, in order to crate all-in-one handheld devices that can be deployed in situ. Still, the fabrication of detailed nanostructures that promote high plasmonic enhancement is challenging, and the creation of metallic nanostructures using microelectrodes and other miniature structures has been a viable alternative. In this work, we present different strategies, based on SERS-active hybrid nanoparticle-nanoaperture structures, as well as 2D and 3D structured nano-topographies, for the detection of analytes of interest.

I065

EXPLORATION OF BIOFILM ATTACHMENT AND GROWTH ON PREMISE PLUMBING MATERIALS THROUGH ATOMIC FORCE MICROSCOPY. **Samuel Collins**[1,2,3], Tianxiao Ma[2], Sarah Jane Payne[1,3], Zhe She[2,3]. [1]Department of Civil Engineering, Queen's University, 58 University Avenue, Kingston, ON K7L 3N9, Canada; [2]Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. [3]The Beaty Water Research Centre, Queen's University, Kingston, ON, K7L 3N6, Canada. (18slc7@queensu.ca)

Biofilms are dynamic and complex communities of bacteria adhered to a surface through a matrix of extracellular polymeric substance (EPS), which improves surface adhesion, protects against environmental stressors, and acts as a communication network at sufficient bacterial density [1]. The (re)growth of biological material is of concern in drinking water distribution systems where biofilms can cause enhanced corrosion of pipe materials and release harmful, sometimes pathogenic, contaminants into the water stream [1, 2]. Conventional techniques to characterize biofilms require the removal of the film from the substrate to evaluate the contents of the matrix (e.g., biological assays, genetic sequencing) or chemical staining to improve imaging of surface structures (e.g., electron and fluorescence microscopy) [1, 2]. Atomic force microscopy (AFM) is used in tapping mode to image the topography of chemically fixed and dried biofilms on their native substrates, providing an accurate snapshot of the surface topography with modified mechanical properties [3]. Biofilms were grown on household plumbing materials (copper and PVC coupons), suspended in beakers of bacterially active feedwater, over a four-week period and extracted bi-weekly to investigate the initial bacterial adhesion, growth of the EPS matrix, and diversity of the biofilm over time.

[1] M.J. Franklin et al., Microbial Biofilms: Second Edition, (2015) 1-32.
[2] S. Kodakkat et al., Methods in Microbiology Vol. 54 (2024) 39-79.
[3] S. James et al., Microbial Biofilms - Importance and Applications (2016) Chapter 6.

I066

DIFFUSION AND ION-EXCHANGE IN LOW-PERMEABILITY ROCKS: LABORATORY-BASED X-RAY SPECTROSCOPY. Charles Cadieux[1], **Tom A. Al**[1], Samuel Morfin[1], Laura Kennell[2]. [1]Department of Earth Sciences, University of Ottawa, Ottawa, ON, Canada. [2]Nuclear Waste Management Organization, 22 St. Clair Avenue East, Toronto, ON M4T 2S3, Canada. (tom.al@uottawa.ca)

The commonly proposed method of long-term storage of radioactive waste in deep geological repositories is based on the premise that the rocks form an effective barrier to solute migration. It follows that groundwater flow must be negligible and rates of solute diffusion in rock porewater must be very low. The rate of solute transport through rocks with immobile porewater is controlled by a combination of diffusion and water-rock reactions, but there are few methods to study these processes in rocks. In this research, a novel energy-dispersive X-ray fluorescence (EDXRF) technique was developed to study simultaneous diffusion of non-reactive (iodide) and reactive (cesium) tracers in rock porewater. Samples of the Queenston Formation shale were obtained from boreholes drilled at the Bruce nuclear site in southwest Ontario, Canada. The method allowed determination of pore diffusion coefficients of $6.1 \text{ +/- } 0.4\times10^{-11}$ m^2/s and $9.5 \text{ +/- } 1.3\times10^{-11}$ m^2/s for I^- and Cs^+, respectively, as well as a cation exchange capacity of 1.8 +/- 0.7 meq/100g and a selectivity coefficient for the exchange of Na^+ for Cs^+ of 2.3 +/- 0.2. This spectroscopic technique represents a versatile new tool for efficient, in-situ study of diffusion and reaction processes in low-permeability rocks.

I067

INVESTIGATING N-HETEROCYCLIC CARBENES ON METAL SURFACES USING ELECTROCHEMICAL AND MICROSCOPIC TECHNIQUES.

K. Wang[1,2]**,** T. Ma[1,2], M. D Aloisio[1,2], C. M. Crudden[1,2], & Z. She[1,2]. [1]Department of Chemistry and [2]Carbon to Metal Coating Institute, Queen's University, Kingston, ON, Canada. (23bq10@queensu.ca)

Self-assembled monolayer (SAM) is a layer of molecules self-assembled onto a surface due to its high binding affinity. Thiol SAM on gold has been the most common due to easy preparation and formation of high density SAM. Recently, N-heterocyclic carbenes (NHCs) have emerged as a promising alternative for forming SAMs, offering higher stability than thiols under most of chemical and electrochemical conditions. Corrosion affects the integrity and lifespan of infrastructure, appliances, and tools, leading to significant economic consequences. In 2019, the direct cost of corrosion in Canada, including expenditures on maintenance and repairs, was estimated to be 2.98% of Canada's gross domestic product. Comparing with traditional surface protection techniques, such as mechanically bonded coating including epoxy coating, NHC-based coating has the advantages of higher coverage, lower dosage and higher fracture toughness. In this presentation, we will describe a novel approach to modifying NHC-based coating to enhance its ability to protect underlying surfaces from corrosion. The resulting coatings were characterized using scanning electron microscopy (SEM) and energy dispersive X-ray spectroscopy (EDX). The findings demonstrated a promising way to significantly enhance protections with modified NHC-based coating.

I068

DEVELOPING ELECTROCHEMICAL BIOSENSORS FOR DETECTING *ESCHERICHIA COLI* AND ANTIBIOTIC-RESISTANT BACTERIA BY MONITORING BIOMOLECULES;

Rebecca X. Y. Chen, Zhe She, R. Stephen Brown; Queen's University Chemistry Department, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (rebecca.chen@queensu.ca)

A contaminant of emerging concern with significant impact on the environment and in clinical settings is antibiotic-resistant bacteria (ARB). The Council of Canadian Academies reported that ARB caused an estimated 14,000 deaths, and expenses attributed to antimicrobial resistance (AMR) cost the Canadian healthcare system $1.4 billion in 2018. In 2019, the CDC reported more than 2.8 million infections and 35,000 deaths caused by AMR in the USA. Current methods for detecting bacteria and ARB rely on trained personnel for in-lab culturing and analytical instrumentation to obtain results after more than 48 hours. These methods cannot be used for rapid, routine testing of ARB nor for on-site real-time monitoring, especially in remote areas. Detecting and monitoring ARB contributes to understanding and characterizing AMR ultimately informing policy. The recent SARS-CoV-2 pandemic demonstrated the efficiency and accessibility of point-of-care self testing. This research addresses the demand for rapid, low-cost, portable, sensitive, and specific detection of ARB. Electrochemical biosensors can detect bacteria and ARB directly, such as by antibody binding, or indirectly as demonstrated effectively in this work by detecting indicator microbe-specific biomolecules. The versatility of biosensor designs presents an opportunity to develop a multiplexed electrochemical device for multiple bacterial and ARB analytes.

I069

AN AMBIENT IONIZATION APPROACH FOR DIRECT, AUTOMATED NATURAL PRODUCTS ASSESSMENT.

Jess Deng, Jian Yu, Jennifer L. Kolwich, Kyla Toshack, Haidy Metwally, Avena Clara Ross, **Richard Oleschuk**. Department of Chemistry, Queen's University, Kingston, ON K7L 3N6, Canada. (oleschuk@queensu.ca)

Ambient ionization methods allow for rapid mass spectrometric analysis with minimal sample preparation. The liquid micro-junction surface sampling probe utilizes a balanced inward and outward flow of a carrier solvent, producing a continuously flushing droplet at the probe tip. Analytes that enter the probe tip through contact/extraction or injection are carried to the electrospray ionization source and ionized in single digit second time frames. The extraction selectivity can be controlled through the composition of the carrier solvent. We present an automated platform to directly profile bacteria and filamentous fungi species (e.g., *Pseudoalteromonas sp*. *Penicillium sp*., and *Trichoderma sp*.) in single organism and multispecies co-cultures. The probe is mounted on a 3-D printer chassis for rastered analysis (*x,y,z*) across the culture allowing for specific colonies to be targeted or the entire plate profiled by altering the sampling pattern. Resulting spectra are subjected to an unsupervised multivariant analysis-driven method to create a hyperspectral image. This method can be used to annotate different *m/z* by straightforward color differences without the need to directly interrogate the spectra. The approach has facilitated the discovery of novel natural products and may be used to monitor changes in expressions with time or growth conditions.

I070

CHARACTERIZING STRUCTURE AND DYNAMICS TO UNDERSTAND AND ENGINEER SPIDER SILK-BASED BIOMATERIALS.

Jan K. Rainey, Dalhousie University, Department of Chemistry, Department of Biochemistry & Molecular Biology, and School of Biomedical Engineering, 5850 College St., Halifax, NS B3H 4R2, Canada. (jan.rainey@dal.ca)

Spider silks are renowned as lightweight materials with outstanding mechanical behaviour, some of which are extremely strong, others extremely extensible, and others still both strong and extensible specifically enabling high energy dissipation. Female orb-weaving spiders produce seven different silk types for different purposes, six of which are fibrillar, each composed of a distinct protein and produced in a specific gland. Fibrous silks proteins are stored in the gland in soluble form at very high concentration and then pultruded to rapidly form insoluble fibres. In this process, silk proteins undergo both structural and self-assembly-state transformations which remain elusive at the atomic level. Here, I will discuss our solution-state NMR spectroscopy studies of structure and dynamics for the storage state of the aciniform (prey wrapping) silk and pyriform (attachment disc) silk proteins, including delineation of protein features enabling structural transformation during fibre spinning and comparing these to our solid-state NMR-based fibrous state structural evaluation. Broader applicability comes both from understanding fundamental properties of fascinating natural materials and through providing the atomic- and molecular-level detail needed to rationally engineer spider silks with desired functional performance. Examples of engineering of silk proteins for distinct function (or dysfunction!) will be detailed.

I071

DETERMINING ANNIHILATION REACTION RATE CONSTANTS OF $Ru(BPY)_3(PF_6)_2$ THROUGH SINGLE ELECTROCHEMILUMINESCENCE (ECL) EVENTS. **Tianyu Wei**, Zhenzhong Cai, Jessica Winslade, Zhifeng Ding. Department of Chemistry, The University of Western Ontario, 1151 Richmond Street, London, ON N6A5B7, Canada. (twei56@uwo.ca)

The annihilation rate constants of Tris(2,2′-bipyridine) ruthenium (II) hexafluorophosphate ($Ru(bpy)_3(PF_6)_2$) were determined by comparing experimental data obtained through single-event electrochemiluminescence (ECL) with simulated results from COMSOL Multiphysics software (version 5.3). In this study, two different three-electrode systems were utilized for comparison. One setup featured a working electrode consisting of a 2 mm platinum disc sealed in a glass tube, while the other employed a platinum ultramicroelectrode (UME) with a diameter of 25 µm. Both systems incorporated platinum coils as counter electrodes and a reference electrode. A 0.1 mmol/L solution of $Ru(bpy)_3(PF_6)_2$ was used in the experiments. The oxidation and reduction potentials of $Ru(bpy)_3^{2+}$ radical ions were determined through cyclic voltammetry (CV) to further analyze the luminescence properties of $Ru(bpy)_3(PF_6)_2$. The application of specific voltages generated $Ru(bpy)_3^{2+}$ cation and anion radicals, which, upon recombination, formed excited-state $Ru(bpy)_3^{2+}$ radicals that emitted photons. These emitted photons were detected using a photon-counting head, and the ECL signal was recorded as a pulse series using an SR430 instrument, which generated a time vs. ECL intensity plot. To simulate the process, COMSOL was used, with one of the key parameters being the diffusion coefficient of $Ru(bpy)_3^{2+}$, determined using the chronoamperometry (CA) technique. The equation $i/id = 1 + 2r\pi^{-3/2}D^{-1/2}t^{-1/2}$ was applied, where i is the current, id is the steady-state current, r represents the radius of the electrode, and t is time. While parameters such as the emission rate constant, quenching rate constant, radical cation decay constant, and radical anion decay constant were held constant, the annihilation rate constants were varied. These were compared to the experimental data from the SR430 instrument. This approach provided a more efficient and accurate determination of the annihilation rate constants.

[1] Quinn, B.; Ding, Z.; Moulton, R.; Bard, A., *Langmuir* **2002**, 18, 1734-1742.
[2] Hesari, M.; Ma, H.; Ding, Z., *Chem. Sci.* **2021**, 12, 14540-14545.

I072

THE IMPORTANCE OF SAMPLE DIGESTION FOR ARSENIC DETERMINATION IN BABY FOOD. **Peter Kettisch**, Anton Paar GmbH, Anton Paar Str. 20, 8053 Graz, Austria.

More than perhaps any other foods, baby and infant foods are subject to close scrutiny for trace metal contamination from cultivation or processing. Low ppb levels of inorganic contaminants such as As, Cd, Pb, Hg and others must be accurately analyzed by ICP-MS. The quality of sample digestion prior to analysis is critical for error-free analysis, with the residual carbon content of the digestion solution being a key parameter. The enhancement of arsenic signals in ICP analysis due to residual carbon, leading to false positives, is a well-known phenomenon.

The US FDA EAM 4.7 method has defined two procedures for sample digestion followed by ICP-MS determination. Criteria for the choice of digestion technology - oven or autoclave digestion - are presented, together with some tips and tricks for optimising sample preparation procedures. ICP-MS results from spike experiments with baby food matrices demonstrate the accuracy and applicability of the method. Particular attention is paid to the accurate determination of arsenic.

I073

DENDRITE FORMATION ON ZINC ELECTRODES IN MILDLY ACIDIC ELECTROLYTES: WHAT CAN WE LEARN USING ELECTROCHEMICAL TECHNIQUES? Andrew J. Sellathurai, Mahmoud Khademi, Bo X. Zhang, Munyah Al-Hamdani, and **Dominik P.J. Barz**, Graphene Integrated Functional Technologies (GIFT), Department of Chemical Engineering, Queen’s University, Kingston, ON K7L 2N9, Canada. (dominik.barz@queensu.ca)

The use of zinc electrodes in mildly acidic aqueous batteries remains challenging, partly because of dendrite formation during charge and discharge cycling. This study investigates the influence of reduced graphene oxide surface coatings and electrolyte additives on the stripping/electroplating performance of zinc. Partially and fully coated electrodes are investigated and compared to the performance of a bare zinc surface. The electrolytes consist of zinc sulphate with sodium sulphate and/or sodium acetate as additives. A series of electrochemical characterization techniques, including cyclic voltammetry, linear sweep voltammetry, electrochemical impedance spectroscopy, chronopotentiometry, and galvanostatic charge and discharge cycling combined with post-mortem scanning electron microscopy is used to characterize the electrode-electrolyte combinations. The results show that the coatings, in combination with a suitable background electrolyte, greatly improve the reversibility and stability of the zinc plating/stripping. A fully coated electrode with a sodium sulphate electrolyte additive achieves almost 450 hours of stable operation before failure. The bare zinc electrode under the same conditions, however, already shows severe voltage fluctuations after around 240 hours. Our comprehensive characterization identifies the influence of the electrochemical (kinetic) parameters on the dendrite formation. The knowledge can be used to derive general rules for the design of electrode-electrolyte interfaces.

I074

CYTOTOXICITY AND METABOLISM OF CdSe/ZnS QUANTUM DOTS. **Bin Hu,** Department of Chemistry, Wuhan University, Wuhan, China, 430072. (binhu@whu.edu.cn)

Due to their unique advantages, quantum dots (QDs) have shown great prospect in clinical application. However, the biosafety of QDs has been a tough question to be answered because of their nano-size effect and heavy-metal components. Hyphenated techniques by combining high-resolution separation technique with sensitive elemental specific detection techniques (eg. inductively coupled plasma mass spectrometry, ICP-MS) and molecular mass detection techniques should be an effective strategy for this purpose, because they can provide the information of the amount, species, distribution, transformation and metabolism of QDs in living cells and organism, which benefits the explanation of the mechanism of toxicity caused by QDs from molecular levels. In this presentation, I will present our preliminary studies on cytotoxicity and metabolism of CdSe/ZnS QDs in HepG2 cells.

[1] Peng L, He M, Chen BB, et al. (2013) *Biomaterials.* 34(37): 9545-9558.
[2] Peng L, He M, Chen BB, et al. (2015) *ACS Nano.* 9(10): 10324-10334.
[3] Chen BB, Peng L, et al. (2023) *Chin. Chem. Lett.* 34: 107262.

I075

BIOACCESSIBILITY AND RISK ASSESSMENT OF Pb, Se, Cd AND Zn FROM SEAWEED.

Helen Lord[1], Kelly LeBlanc[2], Iris Koch[3], Zoltan Mester[2], **Diane Beauchemin[1].** [1]Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; [2]National Research Council of Canada, Metrology Research Centre, 1200 Montreal Rd, Ottawa, ON K1A 0R6, Canada; [3]Environmental Sciences Group, Royal Military College of Canada, Station Forces Kingston, ON K7K 7B4, Canada. (diane.beauchemin@queensu.ca)

Toxic elements (TEs) like Pb, Zn, Cd and Se, depending on their concentrations, are known to contaminate some novel, plant-based protein sources, including seaweed. Using a continuous on-line leaching method (COLM) coupled to an inductively coupled plasma mass spectrometer, the maximum bioaccessible fractions of TEs were determined in a GSEA-1 seaweed certified reference material. Results from the COLM were compared to bioaccessible concentrations measured by a conventional batch method and showed that less than 50% was leached into all gastrointestinal phases for the majority of TEs. Based on TE risk calculations that incorporate bioaccessibility, the hazard quotients (HQs) for Zn and Se were below 0.2, indicating negligible risk for these elements. Under worst-case scenario conditions, HQs were determined to be about 1.0 for Pb and 5.8 for Cd; however, a more realistic ingestion rate revealed that HQs are lower than 1 for Pb, and around 1 for Cd.

I076

ADVANCES IN NANOPARTICLE CHARACTERIZATION USING LASER-ABLATION SINGLE PARTICLE ICP-MS.

Andreas Limbeck, O. Lanaridi, E. Foisner, L. Kronlachner, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, 1060 Vienna, Austria. (andreas.limbeck@tuwien.ac.at)

Over the last decade, single particle inductively coupled plasma mass spectrometry (SP-ICPMS) has emerged as an essential analytical tool for nanoparticle analysis. However, traditional SP-ICP-MS, designed for nanoparticles in suspension, presents challenges related to sample stability, sample introduction efficiency, and potential spectral interferences from the suspension medium. In this work, we present an LA-ICP-MS-based approach for the characterization of nanoparticles. For LA sampling, the particles were embedded in a polymer matrix thin film created using spin coating. To circumvent the need for certified reference materials, we developed a novel calibration strategy that utilizes polymer thin films spiked with defined amounts of the targeted analytes. Applicability of this approach for the determination of the mean nanoparticle composition was demonstrated by analyzing a commercially available nanomaterial with a known sample stoichiometry. Further optimization of this procedure enabled analysis of single particles, introduction of the intact nanoparticles into the ICP-MS resulted in short spikes in the transient signal for each introduced nanoparticle, providing accurate information about the size distribution of the investigated nanoparticles. Finally, a recently reported peak broadening approach has been adapted for single particle analysis using LA-ICP-MS, enabling the analysis of binary nanoparticles with quadrupole instrumentation.

I077

SINGLE PULSE RESPONSE LA-ICP-MS IMAGING WITH QUADRUPOLE INSTRUMENTATION.

Andreas Limbeck, J. Willner, M. Podsednik, D.K. Gibbs, L. Brunnbauer, TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, 1060 Vienna, Austria. (andreas.limbeck@tuwien.ac.at)

In the last years LA-ICP-MS has become an established technique for elemental mapping in a wide range of fields. This has been made possible by instrumental developments which significantly improved the performance of the methodology. With advanced ablation cell designs washout times in the ms range are possible, enhancing sensitivity and reducing time demand for analysis. Increased laser repetition rates enable imaging of large areas with highresolution in a reasonable time. However, so far only ICP-ToF-MS can fully exploit the benefits of measuring the short transient signals generated from single laser pulses. Application of this Single-Pulse-Response concept for multi-element imaging with quadrupole instrumentation is hampered by the sequential detection of targeted isotopes. In this work, we investigate the potential of an ICP-Q-MS with significantly reduced dwell and settling times for multi-element imaging using SPR analysis. The effects of instrumental parameters (cycle time, spot size, peak width) on image quality and image artifacts are evaluated by imaging a ceramic test structure. Finally, the applicability of the SPR-based LA-ICP-Q-MS imaging approach is demonstrated by spatially resolved analysis of four elements in Haematococcus pluvialis cell samples with a pixel acquisition rate of 100 Hz.

I078

HIGH-THROUGHPUT ANALYTICAL TOOLS REVEAL OXYGEN REDOX IN NA-ION BATTERIES, ADVANCED X-RAY SPECTROSCOPIES HELP UNDERSTAND IT.

Eric McCalla. McGill University, Department of Chemistry, Montreal, QC, Canada. (eric.mccalla@mcgill.ca)

There is an on-going need to increase the energy density of Na-ion battery cathodes. One promising way to do this is to engage the anions (oxygen) in the redox processes. Though these processes have been known for about 15 years, designing materials that use anionic redox in a stable manner has been extremely slow as only a very limited number of compositions can be explored. Here, I will demonstrate how combinatorial synthesis and electrochemistry was used to unveil incredibly reversible oxygen redox in a number of doped Na-Mn-O materials [1]. The high-throughput screening involved 52 different dopants and revealed a new mechanism to induce oxygen redox wherein large dopants are introduced into Mn sites and result in destabilization of the neighboring oxygens thereby raising their energy and making them accessible at electrochemical potentials that are practical for batteries. Since then, we have followed up with various X-ray absorption spectroscopies to better understand the nature of the oxygen species [2]. We find that the large dopants help isolate the oxygens thereby preventing oxygen dimers that can lead to oxygen gas release.

[1] S. Jia *et al.* Chem. Mater. 34, 11047 (2022).
[2] S. Jia *et al.* ACS Mater. Letters 7, 1370 (2025).

I079

COLLISION-INDUCED DISSOCIATION (CID)-BASED FRAGMENTATION OF GLYCOSYLATED CHOLESTEROL AND GLYCOSPHINGOLIPIDS TO INTERROGATE A NOVEL TRANSGLYCOSYLATION FUNCTION OF MUTANT GLUCOCEREBROSIDASE IN PARKINSON'S DISEASE. **Steffany A.L. Bennett[1,2] & Thao Nguyen-Tran[1,2]**, Zach Miller[1,2], Miroslava Cuperlovic-Culf [2,3], Rachel Saunders-Pullman[4]. [1]Neurolipidomics Lab, India Taylor Lipidomic Research Platform, and Department of Chemistry and Biomolecular Sciences; [2]Ottawa Institute of Systems Biology, Department of Biochemistry, Microbiology and Immunology, University of Ottawa, Ottawa, ON, Canada; [3]Digital Technologies Research Centre, National Research Council of Canada, Ottawa, ON, Canada; [4]Department of Neurology, Icahn School of Medicine at Mount Sinai and Mount Sinai Beth Israel, New York, NY, USA. SteffanyAnn.Bennett@uottawa.ca)

Variants in *GBA1* represent the largest share of genetic Parkinson's Disease (PD) burden worldwide. *GBA1* encodes the lysosomal beta-glucocerebrosidase enzyme (*GBA1*-GCase) that releases the glucose headgroup from glucosylceramides (β-GlcCers) and glucosylsphingosine (β-GlcSph). We have pursued a second function of *GBA1* and found that the enzyme does not only release glucose from β-GlcCers/GlcSph but also catalyzes the reversible transglycosylation (*GBA1*-TGase) reaction by transferring this sugar and its isomer galactose from β-GlcCers and β-GalCers to cholesterol to form glucosylcholesterol (β-GlcChol) and galactosylcholesterol (β-GalChol). We present here our targeted lipidomic pipeline which detects and quantifies β-GlcChol and β-GalChol in human plasma. Our established lipidomic pipeline consists of nanobore reversed-phase liquid chromatography-electrospray ionization-tandem mass spectrometry (RPLC-ESI-MS/MS) followed by information-dependent-acquisition of enhanced product ion scan (IDA-EPI) for accurate quantification and confident identification of the lipid substrates and products in the *GBA1*-TGase pathway. We also present a novel algorithm which utilizes lipidomic measurements to calculate the strength of targeted metabolic pathway from steady-state lipid abundances. We report here our quantification of β-GlcCers and β-GalCers, as well as β-GlcChol and β-GalChol and show that the expression of *GBA1*-PD variants increases the strength of *GBA1*'s transferase activity (a novel gain of *GBA1* enzymatic function) in human plasma.

I080

OPTIMIZATION OF EXPERIMENTAL CONDITIONS FOR ENHANCED QUADRUPOLE CENTRAL TRANSITION (QCT) NMR SPECTRAL RESOLUTION IN AQUEOUS SOLUTION. **Ziyao Peng** and Gang Wu, Department of Chemistry, Queen's University, Kingston, ON K7L 3N6, Canada (17zy3@queensu.ca)

Quadrupole central transition (QCT) NMR spectroscopy offers a powerful approach for investigating quadrupolar nuclei, such as ^{17}O, in biological macromolecules. Despite its potential, achieving high spectral resolution remains challenging due to their quadrupolar nature. Recent studies have demonstrated that resolution can be significantly improved by optimizing experimental conditions [1, 2]. In particular, performing ^{17}O QCT NMR at very high magnetic fields (e.g., 35.2 T) has resulted in substantial gains in both sensitivity and resolution. Additionally, adjusting factors like solvent viscosity and temperature can effectively control the molecular rotational correlation time (τ_c), which directly influences line widths. Together, these methodological improvements make ^{17}O QCT NMR a more practical and informative tool for probing the structure and dynamics of complex biological macromolecules.

I081

A NEW PREPARATION SYSTEM FOR NOBLE GAS ISOTOPE RATIO DETERMINATION BY STATIC VACUUM MASS SPECTROMETRY **Domokos Gyore**[1,2], Andrew Tait[2], Wyatt MacSorley[1], Peter Stow[1]. [1]Isomass Scientific Inc. Calgary, AB, T2H 3A9, Canada; [2]Scottish Universities Environmental Research Centre, East Kilbride, G75 0QF, Scotland, UK. (Domokos.gyore@isomass.com)

Noble gases (He, Ne, Ar, Kr, and Xe) are exceptional geochemical tracers of crustal fluids due to the various sources of naturally occurring isotopes and their chemical inertness. However, noble gas isotope ratio determinations are analytically challenging and fluid sample preparation remains a time-consuming process. While noble gas mass spectrometry has significantly improved in the last two decades, systems for fluid sample preparation have only witnessed in-house developments with no general efforts towards commercialization. This creates hurdles to standardization and cross-calibration of laboratories internationally and requires considerable financial commitment and significant expertise from noble gas laboratories to develop and commission their own systems. Isomass Scientific Inc. has strategically positioned itself to be the only provider of commercially available Noble Gas Preparation Systems globally since 2022. The System is a single-benched compact unit. It is most suitable to be used in connection with Qtegra platformed ARGUS VI, Helix SFT and Helix MC10K noble gas mass spectrometers, manufactured by Thermo Fisher Scientific. The Noble Gas Preparation System in conjunction with a mass spectrometer allows determination of noble gas amounts and isotopic ratios at high accuracy and precision. This development will make Canada a leader in the analysis of noble gas isotopes.

I082

VOLTAMMETRIC MEASUREMENTS IN A ROOM TEMPERATURE IONIC LIQUID USING SCANNING ELECTROCHEMICAL CELL MICROSCOPY. **Samaneh Salek,** Joshua C. Byers, Département de Chimie, Université du Québec à Montréal, Montréal, QC, Canada. (salek_esfahani.samaneh@courrier.uqam.ca)

SECCM employs a pipet probe to create a small meniscus cell, enabling high-resolution and localized analysis [1]. Room Temperature Ionic Liquids (RTILs), with their high viscosity and low vapor pressure, provide a stable droplet at the pipet tip, making them ideal for SECCM [2]. This technique has been applied to various electrode materials. However, understanding mass transport in RTILs is critical, as the high viscosity affects the diffusion of redox species and the voltammetric response. While microelectrodes have been used to achieve steady-state voltammetry in RTILs, similar investigations using SECCM are limited. In this study, the effect of pipet diameter on mass transport was examined using ferrocene in 1-ethyl-3-methylimidazolium tetrafluoroborate. Experimental findings, supported by finite element simulations and analytical modeling, demonstrate that under the right conditions, SECCM can achieve steady-state behavior, enabling the determination of key kinetic parameters such as the diffusion coefficient and heterogeneous rate constant on glassy carbon. These results establish SECCM as a reliable and reproducible technique for probing electrochemical kinetics in viscous ionic liquid environments.

[1] Bentley, C.L., et al. *Anal. Chem.*, 2019. 91(1): p. 84-108.
[2] Bentley, C.L., M. Kang, and P.R. Unwin. *Anal. Chem*, 2020. 92(17): p. 11673-11680.

I083

KINETIC ANALYSIS OF PYROLYTIC OIL HEAT TREATMENT WITH MASS SPECTROMETRY. **Simon Laliberté-Riverin**, Marie Aimée Tuyizere Flora, and Houshang Alamdari. Aluminium Research Center – REGAL, Université Laval, Department of Mining, Metallurgical and Materials Engineering, 1065 ave de la Médecine, Québec, QC G1V 0A6, Canada. (simon.laliberte-riverin@gmn.ulaval.ca)

Pyrolytic oil obtained by fast pyrolysis of biomass is a potential precursor for the fabrication of renewable carbon electrode binders. Pyrolytic oil must be heat-treated to provide it with thermoplastic properties necessary for its use as a binder. In the current research we analyze the volatile substances evolved during this heat-treatment process. Oil samples are placed in a reactor and heated to 250 °C at a constant heating rate. Oil mass loss is measured continuously and the atmosphere inside the reactor is sampled by an online quadrupole mass spectrometer. Time series data of mass channels are deconvoluted with principal component analysis. The analysis reveals distinct volatile evolution kinetics for 2 phases: one phase rich in water and oxygen, and the other phase rich in carbon. Those results enable future optimization of the heat treatment process by tuning heat treatment parameters for eliminating the aqueous phase while keeping the carbon-rich one.

I084

UNVEILING THE ROLE OF INTRINSICALLY DISORDERED MOTIFS IN P97-P47 COMPLEX USING SOLUTION NMR SPECTROSCOPY. **Rui Huang.** University of Guelph, Guelph, ON, Canada. (rhuang08@uoguelph.ca)

Cellular activities reply on proper functioning of a myriad of large biomolecular complexes. To understand the mechanisms by which these molecular machines work, it is crucial to obtain structural information as well as detailed characterization of their conformational dynamics. Here we present our structural study characterizing the dynamic complex formed between p47 and a 320-kDa p97 construct using solution Nuclear Magnetic Resonance (NMR) Spectroscopy. p97 is a highly conserved and abundant cytosolic enzyme in the AAA+ superfamily (ATPases associated with diverse cellular activities). It plays an indispensable role in protein homeostasis and is involved in a variety of diverse cellular processes ranging from proteasomal and lysosomal degradation to membrane fusion and cell cycle regulation. Elevated expression of p97 has been reported in a number of different cancer types and is correlated with cancer aggressiveness and therapeutic resistance, making p97 a promising therapeutic target. p97 interacts with more than 30 adaptor proteins which recruit p97 to various specific cellular functions, one of which, named p47, directs p97 function to the remodelling of cellular membranes. We discovered multiple previously unidentified linear motifs residing in the intrinsically disordered linker region of p47 that play important structural and functional roles in the complex. We characterized the intra-molecular and the inter-molecular interactions involving these motifs, and demonstrated how these interactions are regulated by the nucleotide state of p97 and dictate the overall dynamics and functionality of the complex. Our results highlight the important roles that intrinsically disordered regions (IDRs) play in regulating the structure and function of large molecular assemblies.

I085 P

TOUCH-AND-GO METABOLOMICS FOR FUNGAL NATURAL PRODUCTS. **Jessie F. Deng**, Jennifer L. Kolwich, Avena C. Ross, Richard D. Oleschuk, Department of Chemistry, Queen's University, Kingston, On, Canada. (j.deng@queensu.ca0

Natural Product (NP) discovery is often hindered by laborious extraction, chromatography and structure elucidation workflows. To address this inefficiency, we developed a rapid, minimally invasive metabolomics pre-screening pipeline using the Liquid Microjunction Surface Sampling Probe (LMJ-SSP) coupled with mass spectrometry and molecular networking. This approach enables the direct surface analysis of fungal colonies within seconds, providing chemically rich profiles with minimal sample preparation. Applied to Penicillium species, the LMJ-SSP platform allowed quick dereplication (within minutes) of known metabolites and detection of structurally related analogs using the Global Natural Products Social Molecular Networking Platform (GNPS). Comparative analysis with conventional LC-MS/MS confirmed that the LMJ-SSP captured the most abundant and chemically informative signals, validating its use as a pre-screening tool. This workflow functions as an intelligent triaging step, guiding targeted isolation efforts and minimizing redundancy. It offers a non-destructive strategy to inform downstream chromatographic fractionation, saving time and resources. The LMJ-SSP represents a versatile and efficient front-end to NP discovery workflows and had broad potential for application across other microbial and plant systems.

I086

ADSORPTION SELECTIVITY AND DEFECT ENGINEERING IN METAL-ORGANIC FRAMEWORKS: INSIGHTS FROM SSNMR. **Yining Huang**,[1] Tahereh Azizivahed,[1] Anupom Roy, [1] Mikko Karttunen,[1] Jiabin Xu,[1,2] Jun Zhong,[2] Tsun-Kong Sham.[1] [1]Western University, Department of Chemistry, 1151Richmond Street, London, ON N6A 3K7 Canada1; [2]Institute of Functional Nano and Soft Materials Laboratory (FUNSOM), Soochow University, Suzhou 215123, China (yhuang@uwo.ca).

Metal-organic frameworks (MOFs) are tunable porous materials with diverse applications. Understanding adsorption selectivity and defect formation at the molecular level is key to optimizing performance.

Efficient C_2H_2/CO_2 separation is critical for industrial gas purification, as both gases have similar properties. This study examines their selective adsorption in microporous MOFs using solid-state NMR (SSNMR), quantum mechanical modeling, and molecular dynamics simulations. The MOFs SIFSIX-1-Cu and SIFSIX-3-Cu share the same topology but differ in the length of their organic linkers. They exhibit distinct behavior toward C_2H_2 and CO_2. In-situ variable-temperature ^{13}C and ^{2}H SSNMR along with ab initio calculations reveal SIFSIX-1-Cu prefers C_2H_2, while SIFSIX-3-Cu adsorbs both gases efficiently.

Defect engineering modifies MOF properties. Here, missing cluster and linker defects are introduced into Zr-UiO-66 using trifluoroacetic acid (TFA) as a modulator. Multinuclear SSNMR (^{1}H, ^{13}C, ^{19}F, ^{91}Zr, ^{35}Cl, ^{17}O) and in situ XAFS at the Zr K-edge probe defects and structural changes during TFA removal. These defects enhance Pt nanoparticle catalysis in the hydrogen evolution reaction (HER), with defective Pt-UiO-66 outperforming non-defective Pt-UiO-66 and commercial Pt/C.

I087

QUADRUPOLE-CENTRAL-TRANSITION NMR SPECTROSCOPY OF LOW-GAMMA QUADRUPOLAR NUCLEI.

Gang Wu. Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (wugang@queensu.ca)

Quadrupole-central-transition (QCT) NMR spectroscopy utilizes the special quadrupole relaxation properties of the so-called central transition (CT) for half-integer quadrupolar nuclei with half-integer spins in the slow motion regime [1]. To date, successful QCT NMR studies have been reported in the literature for studying ^{17}O (I = 5/2) [1], ^{23}Na (I = 3/2) [2], ^{27}Al (I = 5/2) [3], ^{51}V (I = 7/2) [4], ^{59}Co (I = 7/2) [5] and ^{87}Rb (I = 3/2) [6]. In this presentation, we will explore the feasibility of QCT NMR studies for notoriously difficult low-gamma quadrupolar nuclei such as ^{39}K (I = 3/2), ^{25}Mg (I = 5/2), and ^{67}Zn (I = 5/2).

[1] G. Wu, *Prog. Nucl. Magn. Reson. Spectrosc*. 114/115 (2019) 135.
[2] J. Zhu, G. Wu, *J. Am. Chem. Soc*. 133 (2011) 920.
[3] J. M. Aramini, M. W. Germann, H. J. Vogel, J. Am. Chem. Soc. 115 (1993) 9750.
[4] A. Butler, H. Eckert, *J. Am. Chem. Soc*. 111 (1989) 2802.
[5] J. Shen, V. Terskikh, G. Wu, *ChemPhysChem* 20 (2019) 268.
[6] Z. Peng, G. Wu, *J. Phys. Chem. A* 129 (2025) 803.

I088 P

MONITORING SPATIOTEMPORAL DYNAMICS OF MICROBE CO-CULTURE METABOLITES USING AMBIENT MASS SPECTROMETRY.

Jennifer L. Kolwich, Jessie F. Deng, Kyla M. Toshack, Richard D. Oleschuk, Avena C. Ross. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (jennifer.kolwich@queensu.ca)

Soil harbors complex microbial communities where interactions are mediated by diverse secreted chemicals. Microbes are often cultured in close contact, or "co-cultured", to mimic these community interactions. Chemically mapping these dynamics provides insight into metabolite-based interactions and helps prioritize isolation of bioactive molecules. However, conventional chemical analysis methods, like bulk solvent extraction, are destructive and often lose rich spatiotemporal data, while common mass spectrometry imaging techniques have sample preparation or surface-feature requirements that make it challenging to map metabolites on the same sample over time. This work uses the liquid microjunction surface sampling probe paired with a triple quadrupole mass spectrometer to spatiotemporally map metabolites of isolated and co-cultured soil microbes in custom chambers modeling micro-ecological interactions.

Using this method, metabolite profiles were obtained over several days to track changes in activity along the surface of growing microbes and surrounding agar, revealing the molecular interplay between the co-cultured organisms. We observed the initial production and movement of known microbial metabolites, like griseofulvin analogues and prodiginines, and novel compound masses correlated with microbial interaction zones. Overall, this tool provides a robust, preparation-free method for mapping microbial metabolite dynamics, enabling mechanistic insight into microbial ecology and informing natural product isolation and discovery.

I089

LITHIUM QUANTIFICATION BY LASER INDUCED BREAKDOWN SPECTROSCOPY.

Silum Ghebreyesus, Mariam Coulibaly, Jonathan Côté, Marc Constantin, Jocelyn Bouchard. Université Laval, Département de géologie et de génie géologique, 1065 Ave de la Médecine, Québec, QC G1V 0A6, Canada. (silum.ghebreyesus.1@ulaval.ca)

With the growing demand for battery technologies, lithium has become a critical element in the global energy transition. However, its low atomic number renders it undetectable by conventional X-ray fluorescence (XRF), positioning Laser-Induced Breakdown Spectroscopy (LIBS) as a promising alternative for lithium exploration. This study employed LIBS measurements on pressed powder pellets prepared from certified reference materials (CRMs) of lithium-bearing pegmatites with known elemental compositions. Spectral peaks were identified using an automated peak detection algorithm and modeled using Partial Least Squares Regression (PLSR) to capture consistent emission features across all spectra. Key predictors from the PLSR model were refined using ridge regression with a penalty to reduce multicollinearity and suppress less informative variables. Only the final sparse ridge regression model was kept for lithium quantification in unknown samples, including pulverized materials from metallurgical products, run-of-mine ore, borehole cuttings. Model predictions were validated against conventional chemical analyses, confirming that the LIBS-based workflow enables rapid, accurate, and field-deployable quantification of lithium. The overall methodology integrates spectral averaging, automated peak extraction, and a two-stage multivariate modeling approach to enhance predictive robustness and isolate lithium-relevant spectral features.

I090

INFRARED-HEATED TOTAL CONSUMPTION SAMPLE INTRODUCTION SYSTEM FOR THE ANALYSIS OF COMPLEX GEOLOGICAL SAMPLES BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY.

William Hachey and Diane Beauchemin. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (17wrjh@queensu.ca)

The Canadian mineral sector must rely heavily on analytical chemistry when identifying and quantifying minerals. A popular analytical tool used to analyze geological samples is inductively coupled plasma mass spectrometry (ICPMS). This technique can instantaneously measure multiple elements with, depending on the analyte and matrix, a detection limit as low as one part per quadrillion. However, the system has a low sample transport efficiency, and the noise of the nebulization process affects the detection limit. These limitations can be overcome by using an infrared (IR)-heated sample introduction system to pre-evaporate the sample and reduce the droplet size so more enters the ICP while decreasing the noise accompanied by nebulization.[1] This work centers on optimizing an IR-heated total consumption sample introduction system for the analysis of geological samples with complex matrices. The effect of IR heating on sensitivity, detection limit, robustness, and spectroscopic interferences in ICPMS is examined. This research will benefit the analytical services industry by enhancing mineral analysis results while cutting waste disposal costs.

[1] Al Hejami, A.; Burgener, M. J.; Burgener, J.; Beauchemin, D. *J. Anal. At. Spectrom.* **2020**, *35* (6).

I091

ION CHROMATOGRAPHIC SAMPLE INTRODUCTION INTO ICP-MS/MS AND APPLICATION TO RADIOACTIVE NUCLIDES ANALYSIS. **Yoshitaka Takagai**[1]*, Kayo Yanagisawa[1,2], Makoto Matsueda[1,3], and Makoto Furukawa[1,4]. [1]Fukushima University, Cluster of Science and Technology, 1 Kanayagawa, Fukushima 960-1296, Japan; [2]Japan Atomic Energy Agency, Nuclear Science and Engineering Center, Research Group for Nuclear Chemistry, 2-4 Shirakata, Tokai, Ibaraki 319-1195, Japan; [3]Japan Atomic Energy Agency, Collaborative Laboratories for Advanced Decommissioning Science, 10-2 Fukasaku, Miharu, Fukushima 963-7700, Japan; [4]PerkinElmer Japan G.K., 1-1-32 Shinurashima-cho, Kanagawa-ku, Yokohama, Kanagawa 221-0031, Japan. (s015@ipc.fukushima-u.ac.jp)

Information on radionuclides derived from inorganic mass spectrometry is valuable for environmental monitoring, radiation dose assessment, nuclear waste management, decommissioning, dating, tracer studies in biology, medicine and geochemistry. ICP-MS(/MS) is a highly sensitive and selective method and has been applied to radionuclide analysis by interfacing with various types of sample introduction techniques (e.g. concentric nebulization, ultrasonic nebulization, hydride generation, laser ablation etc.). Although each technique combined with ICP-MS is now well developed, its practical application in the nuclear field is still evolving. We have recently developed an ion chromatography (IC) with ICP-MS/MS. It may seem that techniques like high-performance liquid chromatography-ICP-MS/MS can be used easily, but there is an issue with having to remove ions such as Na and K from the eluent in IC. This technique allows simultaneous removing the matrix ions such Na^+ and K^+, thus extending the potential of ICP-MS in radionuclide analysis. The difficult-to-measure radionuclides were directly automatic-quantified.

I092

A UNIVERSAL AND COST-EFFECTIVE METHOD FOR THE MITIGATION OF INTERFERENCES IN INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Michael Trolio** and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (17mgat@queensu.ca)

Since the conception of the inductively coupled plasma mass spectrometer, polyatomic interferences, the combinations of atoms that produce mass-to-charge ratios which overlap analytical signals, have long decreased method accuracy, sensitivity, and precision. Current mitigation techniques are often selective to the type of interference (oxide, nitrogen, argide, etc) or are too costly for analytical facilities to implement (ex. sector-field, tandem MS). A polyatomic interference method that is universal, cheap, and easy to implement would prove valuable to all affected ICPMS users. This work proposes a low-volume sample uptake method that can universally mitigate polyatomic interferences. The basis of this mitigation method relies on reducing energy spent on non-ionization processes (ex. evaporation, desolvation, atomization, excitation) through the introduction of smaller sample volumes into the plasma, leaving more energy for complete ionization. This work will be expanded to include non-oxide interferences, as well as be combined with mixed-gas plasmas to facilitate a greater transfer of plasma energy to analytes.

I093

MULTI-ELEMENTAL ANALYSIS OF DYED HAIR USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY FOR SEX DETERMINATION. **Chloe Wheeler**, Eleanor Bird, and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (18clw1@queensu.ca)

This research builds upon a previously modified method using electrothermal vaporization inductively coupled plasma optical emission spectroscopy (ETV-ICP-OES) for human sex determination by directly analyzing hair samples.[1] This study and review examines how dyeing alters elemental composition, as an exogenous factor, evaluates the modified method's effectiveness under these conditions, and extends this method to chemically altered (dyed) head hair. To account for sample loading effects on the plasma, an argon emission line is used for point-by-point internal standardization, followed by background correction, peak area integration, and multivariate analysis using principal component analysis (PCA) and linear discriminant analysis (LDA). The predictor elements were changed to include Cd, Fe, Ca, and Sr, allowing accurate sex determination of humans from dyed and undyed hair samples. Ultimately, this study presents a more robust, green chemistry-based model that uses a cost-effective and accessible carrier agent, expanding the method's applicability in forensic analysis.

[1] Wheeler, C.; Beauchemin, D. Atomic Spectroscopy 2024, 45(5), 391-399.

I094

ENHANCING CELL SAMPLE TRANSPORT EFFICIENCY USING AN OPTIMIZED INFRARED-HEATED SAMPLE INTRODUCTION SYSTEM FOR YEAST CELL ANALYSIS BY SINGLE-CELL INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY, **Zichao Zhou[1]**, Diane Beauchemin[1], Mirah J. Burgener[2], John Burgener[2]. [1]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; Burgener Research Inc. Burgener Research Inc., 1680-2 Lakeshore Rd. W, Mississauga, ON L5J 1J5, Canada. (16zz39@queensu.ca)

Single-cell ICPMS (scICPMS) enables elemental analysis at the cellular level, but its sensitivity is often limited by low transport efficiency (TE). Enhancing TE is critical for maximizing detection capability and minimizing sample consumption, particularly when working with rare or valuable cells [1]. Total-consumption systems have shown promise, achieving 100% TE for nanoparticles using infrared (IR)-heated spray chambers [2]. However, due to the larger size and different thermal tolerance of cells compared to nanoparticles, these optimized conditions are not directly applicable to scICPMS. In this work, an IR-heated sample introduction system with a SC175 nebulizer was optimized for yeast cell analysis by varying temperature, sample uptake rate, sampling position, and nebulizer gas flow rate. Yeast cells and selenium-enriched yeast were used to assess sensitivity for both intrinsic (K, Mg) and target (Se) elements. At 85 °C, a significantly higher number of cell events was detected compared to a standard cyclonic spray chamber at room temperature, indicating improved TE.

[1] M. Corte-Rodríguez, R. Álvarez-Fernández, P. García-Cancela, M. Montes-Bayón and J. Bettmer, *Trends Anal. Chem.*, **2020**, 132, 116042.
[2] Z. Zhou, M. J. Burgener, J. Burgener and D. Beauchemin, *J. Anal. At. Spectrom.*, **2024**, 39, 2078–2086.

I095

NMR METABOLOMICS AND 19-F NMR TO STUDY PER- AND POLYFLUOROALKYL SUBSTANCES IN THE ENVIRONMENT AND BIOLOGICAL SAMPLES.

Lindsay S. Cahill, Memorial University of Newfoundland, Department of Chemistry, 45 Arctic Avenue, St. John's, NL, A1C 5S7, Canada. (lcahill@mun.ca)

Per- and polyfluoroalkyl substances (PFAS) are a class of persistent organic pollutants that are used in a variety of products including cookware, cosmetics and firefighting foams. Legacy PFAS (e.g., perfluorooctanoic acid, PFOA) have been banned following the link to numerous health issues. However, these "forever chemicals" remain in the environment and can be found in the blood of all living organisms, potentially causing adverse health effects at all stages of life. Our group recently detected fluorotelomer (FTEOs), a novel class of PFAS, in dust samples taken from healthcare facilities and in industrial wastewater. The toxicity of these novel compounds is unknown. Using experimental mice and ^{1}H high-resolution magic angle spinning NMR, we investigated the impact of PFAS on placental and adult brain metabolism. We also used ^{19}F NMR to detect PFAS in surface ground water near a contamination site in Newfoundland, Canada and in murine tissue samples following PFAS exposure through drinking water.

I096

NONLINEAR OPTICAL IMAGING FOR BIOMATERIAL ANALYSIS AND OPTICAL NANOSCOPY.

MacAulay Harvey[1], Richard Cisek[1], Laurent Kreplak[2], and Danielle Tokarz[1]. [1]Saint Mary's University, Department of Chemistry, Halifax, NS, B3H C3C. [2]Dalhousie University, Department of Physics and Atmospheric Science and School of Biomedical Engineering, Halifax, NS, B3H 4J5. (MacAulay.Harvey@smu.ca)

Nonlinear optical imaging is a powerful class of analytical techniques that enable high-resolution, high-sensitivity measurements of molecular structure and hierarchical organization within biological and synthetic materials. In this work, we apply polarization-resolved second harmonic generation microscopy (PSHG), a nonlinear imaging method for probing local protein structure, to investigate the molecular architecture and mechanical behavior of biomaterials.

First, we demonstrate experimentally that the mechanical response of individual collagen fibrils is governed by the spring-like extension of triple-helical collagen molecules. Furthermore, we identify distinct molecular-scale responses to strain between fibrils derived from functionally different tissues. Second, we present the first combined theoretical and experimental application of PSHG to determine the local orientation of β-sheets in silk fibers. Lastly, we introduce recent advances in super-resolution nonlinear optical imaging, achieving spatial resolution up to three times greater than conventional optical imaging methods. This approach enables detailed molecular characterization of biological and synthetic nanostructures beyond the diffraction limit. Together, these findings highlight the versatility and power of nonlinear optical imaging for advancing our understanding of biomaterial structure and mechanics at the nano and molecular scale.

I097

HOW LIGANDS BIND TO GUANINE QUADRUPLEXES. **Anthony Mittermaier**, McGill University, Department of Chemistry, 801 Sherbrooke Street West, Montreal, QC H3A 0B8, Canada. (anthony.mittermaier@mcgill.ca)

Guanine quadruplexes (G4s) are non-canonical, 4-stranded secondary structures formed by guanine-rich nucleic acids that are believed to modulate DNA replication, gene expression, and telomere maintenance. This makes them promising targets for small molecule anti-cancer therapeutics. However, efforts to develop G4-targeting drugs face significant challenges due to limited structural diversity and complex and poorly understood binding mechanisms. We have explored the interaction between the well-characterized small molecule ligand TMPyP4 and a G4 from the promoter region of c-myc, which has been shown to regulate expression levels of this oncogene. We used relaxation dispersion NMR experiments to quantify ligand association and dissociation rates with atomic resolution. Surprisingly, we found that TMPyP4 dissociates from G4s very slowly but can transfer directly among G4s and between G4s and double-stranded DNA rapidly. This "direct transfer" mechanism parallels reduced-dimensional diffusion processes observed in protein-DNA interactions but has not previously been reported for G4s. By facilitating the escape from off-target binding events it could accelerate target acquisition in the cell, potentially improving the specificity and efficiency of G4-targeting therapeutics.

I098

ATOMIC INSIGHTS: SOLID-STATE NMR ACROSS THE MOF LANDSCAPE. **Yining Huang**. Western University, Department of Chemistry, 1151Richmond Street, London, ON N6A 3K7 Canada. (yhuang@uwo.ca).

Metal-organic frameworks (MOFs) have emerged as the largest and most versatile class of porous materials with numerous applications. Despite their widespread utility, many fundamental questions remain, particularly regarding the precise architectures, electronic environments, and behavior of guest molecules. Solid-state NMR (SSNMR) provides an invaluable tool for investigating these features at the atomic level. MOFs incorporate elements from across the periodic table, including numerous challenging quadrupolar nuclei. We have pushed the boundaries of both high-resolution and wideline SSNMR of quadrupolar nuclei, employing state-of-the-art technologies for MOF characterization. We have examined diverse metal environments in MOFs such as ^{67}Zn, ^{25}Mg, ^{115}In, ^{91}Zr, $^{71/69}$Ga, ^{139}La, ^{43}Ca, $^{47/49}$Ti, $^{63/65}$Cu, ^{209}Bi *etc*., uncovering detailed insights into metal coordination and local bonding environments. In addition to conventional ^{1}H and ^{13}C SSNMR, we have expanded linker characterization to include ^{17}O SSNMR, providing a more complete view of the local structures. Furthermore, the behavior of adsorbed guest molecules has been directly monitored using SSNMR. Given the breadth of systems studied, only selected examples can be discussed here due to time constraints. Nonetheless, by integrating insights from metals, linkers, and guest species, we demonstrate how SSNMR advances our understanding of structure–property relationships and informs the rational design of next-generation MOFs.

I099

MASS TRANSPORT AT THROUGH AN ELECTROACTIVE BACTERIAL BIOFILM. Nastaran Khodaparastasgarabad, Manon Couture, **Jesse Greener.** Département de chimie, Université Laval, 1045 avenue de la médecine, Québec G1V 0A6, Canada. (jesse.greener@chm.ulaval.ca)

Electroactive biofilms (EABs) formed by *Geobacter sulfurreducens* enable bioelectrochemical systems (BES) to convert chemical energy into electrical current. While much research has focused on electron transfer mechanisms, we demonstrate that mass transport—specifically the flow of substrates like acetate and by-products such as protons—plays an equally critical role in limiting or enhancing performance over time. Using advanced microfluidic devices with integrated 3-electrode control and precise modulation of flow, temperature, and substrate concentration, we studied how metabolic bottlenecks evolve in EABs during long-term growth. Early-stage activity is constrained by electron transfer through cytochromes, but as biofilms mature, the dominant limitation shifts to enzymatic substrate oxidation, driven by changes in permeability and apparent enzyme affinity ($K_{M(app)}$). Flow mode and rate were found to strongly influence acetate access and proton removal, particularly in aging biofilms, leading to record-high current densities (>29 A m^{-2}) in microfluidic systems. These results highlight the central role of chemical mass transport within the EAB and suggest that tuning flow and substrate delivery can strategically shift rate-limiting steps, providing a new experimental roadmap for BES optimization.

I100

PHOTONIC-BASED MULTI-GAS SENSOR FOR CONTINUOUS MONITORING OF COMPLEX GAS MIXTURE, **Simon Dallaire**[1], Antoine Hamel[1], Ross Cheriton[2], John Weber[2], Martin Vachon[2], Shurui Wang[2], Dan-Xia Xu[2], Pavel Cheben[2], Siegfried Janz[2], Jens H. Schmid[2], Francis Vanier[1], Daniel Gagnon[1], Mohamad Sabsabi[1], [1]National Research Council Canada – Clean Energy Innovation Research Centre, 75 de Mortagne, Boucherville, Canada, [2]National Research Council Canada – Quantum and Nanotechnologies Research Center, 1200 Montreal Road, Ottawa, Canada.

This project aims to develop and scale a photonic-chip-based multi-gas sensor for industrial applications, focusing on continuous monitoring of complex gas mixtures. The sensor integrates a patented NRC spectral correlation photonic chip designed for remote sensing of gases by analyzing their spectral fingerprints. Light is filtered through a tunable micro-ring resonator on the chip, allowing for targeting multiple gases due to the chip's compact size. The system includes modules for illumination, detection, and communication, making it adaptable for IoT applications. Initial testing showed high coupling loss, yet the sensor detected a signal with remaining light, indicating potential for quantification improvements. Tests using CO_2 mixtures demonstrated the sensor's capability in laboratory settings, achieving a sensitivity level suitable for detecting various gases. Future steps involve enhancing the system's electronics and algorithms, integrating the sensor into NRC's Anaerobic Bioprocessing pilot plant for real-world conditions, and confirming minimal maintenance and reliability in harsh environments.

I101

TRANSFER AND PERSISTENCE OF GSR ON FABRICS: MP-AES AND ICP-MS ANALYSES. Mikala Beaule[1], Deanna Haas[1], Dr. Shannon Accettone[1,2], Dr. David Ruddell[3], Dr. **Sanela Martic**[1,4]. [1]Department of Forensic Science, Trent University, Peterborough, ON, Canada, [2]Department of Chemistry, Trent University, Peterborough, ON, Canada, [3]Center of Forensic Sciences, Toronto, ON, Canada, [4]Trent School of Environment, Environmental Life Sciences, Materials Science Program, Water Quality Center, Trent University, Peterborough, ON, Canada. (sanelamartic@trentu.ca)

Gunshot residue (GSR) is emitted from a firearm and deposits on the nearby surfaces. The presence of lead, barium, and antimony is characteristic of GSR particles, however the transfer and persistence of GSR particles make GSR interpretation challenging. Specifically, the fabrics are characterized with various levels of sheddability which influences sampling, persistence and transfer of GSR. Herein, the GSR transfer and persistence on various fabrics were evaluated using MP-AES and ICP-MS methods. The GSR samples were generated by a single shot event using a rifle or a handgun, followed by wiping the weapon with the fabric. Digested fabrics were subsequently analyzed using the two methods, with the ICP-MS exhibiting a higher sensitivity over MP-AES. In addition, the intra-transfer and inter-transfer of GSR on fabrics were also evaluated. The extent of transfer and persistence was also evaluated as a function of fabric type and contact time. The metal deposition heat maps were generated for fabrics to monitor GSR localization on the fabrics, and metal concentrations quantified. All three metals were found on fabrics, but the amount of transfer was highly dependent on the fabric type, and contact time. Data provide insight into the GSR transfer and persistence which is of value to forensic scientists in terms of activity level details and crime scene reconstruction.

I102

MILESTONE'S ULTRAWAVE 3: THE MOST ADVANCED MICROWAVE DIGESTION SYSTEM TO DATE. **Geoff Williams**, ATS Scientific, 4030 Mainway, Burlington, ON L7M 4B9, Canada. (gwilliams@ats-scientific.com)

The Milestone UltraWAVE 3 represents a significant advancement in microwave digestion technology, offering unmatched speed, efficiency, and flexibility for elemental analysis. Utilizing patented Single Reaction Chamber (SRC) technology, the system enables the simultaneous digestion of up to 40 samples with varying matrices and acid chemistries in a single run, eliminating the need for batching and significantly increasing throughput. Operating at temperatures up to 300°C and pressures up to 199 bar, while being capable of doing so for multiple hours, the UltraWAVE 3 ensures complete digestion of even the most challenging sample types. Automated features such as vial sealing, chamber venting, and rapid cooling reduce operator intervention by up to 50%, enhancing safety and efficiency. This combination of speed, and the most complete digestions, make the UltraWAVE 3 the most advanced microwave available on the market.

I103

DEVELOPING MULTIPLEXED ELECTROANALYTICAL METHODS FOR DETECTION OF CONTAMINANTS OF EMERGING CONCERN IN WATER.

Zhe She, Department of Chemistry, Queen's University, Kingston, ON, Canada. (zhe.she@queensu.ca)

Water resources are an essential part of our society and global ecosystem. Understanding how pollutants move through groundwater, environmental water, wastewater and drinking water are critical to protecting both human and environmental health. Contaminants of emerging concern can be either new chemicals or legacy chemicals that are hazardous to human and/or environmental health. There is lack of practical technologies to monitor these contaminants. Monitoring is not only important for detecting these contaminants, in order to avoid consuming contaminated water sources, but also tracking and understanding their dynamics in the water systems, so we can develop effective decontamination and treatment technologies. In our lab, we are interested in electrochemistry and applying it to the development of new methods for detection and identification of hazardous chemicals. In this presentation, I will share the story of our work in multiplexed electrochemical detections and electrode fabrication. [1,2]

[1] Lamothe, N.; Elliott, K.; Pei, Y.; Shi, Y.; Macdonald, K.; Payne, S.J.*; She, Z.*, Electrocatalysis, 2024, 15, 353-362.
[2] Shi, Y.; Pei, Y.; Lamothe, N.; Macdonald, K.; Payne, S.J.*; She, Z.*, ELISA, 2024, 4(3) e2300011.

I104

IMPACTS OF DILUENT MATERIALS ON GAS-PHASE CATALYTIC ACTIVITY.

Lucan Clair, Emerson MacNeil, **Paul Duchesne**, Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada. (paul.duchesne@queensu.ca)

In recent years, increasing focus has been placed on *in situ* and *operando* studies of gas-phase heterogeneous catalyst materials. This is due in large part to observations that the initial material placed into a catalytic reactor can differ greatly in both structure and composition from the active form generated under catalytic reaction conditions (*i.e.*, elevated temperature, increased temperature, reducing atmosphere, *etc.*). XANES and EXAFS analyses offer excellent functionality in this regard, as the high penetrating power of X-rays enables them to pass through the catalytic reaction cell, allowing for truly *in situ* and *operando* characterization. For such experiments, it is common to employ relatively "X-ray transparent" diluents such as boron nitride to achieve optimal X-ray absorption signal. However, initial studies have further revealed that the presence of boron nitride alters the products resulting from the catalyst material. In order to better explore and understand this phenomenon, X-ray photoelectron spectroscopy has been used to study the evolution of catalyst composition and speciation under catalytic reaction conditions. Changes in oxidation state and product gas composition are explored for a series of common gas-phase heterogeneous catalyst materials, affording insight into the processes responsible for this change in catalytic behaviour.

I105

TRANSLATIONAL APPLICATION OF NANOSTRUCTURED BIOSENSORS: DIAGNOSTICS AT THE POINT OF CARE.

Sara Mahshid, Department of Bioengineering, McGill University, Montreal, Quebec, Canada. (sara.mahshid@mcgill.ca)

Development of diagnostic devices with clinically relevant sensitivity and rapidity is highly desirable for decreasing the delay between diagnosis and treatment. Diagnostic inefficiency permeates multiple medical fields, including infectious diseases and antimicrobial resistance (both recognized by WHO among paramount threats and research priorities). Molecular detection is also central to cancer, where therapies are often out of step with disease complexity and progression. The respective challenges may be addressed through the application of nanomaterials and high-throughput devices that offer unique advantages. In Mahshid Lab, we develop novel paradigms in point-of-care diagnosis via synergistically combining innovative nanostructured sensors with fluidic sample delivery systems and analytical assays and spectroscopy approaches. From an engineering perspective, the lab seeks to use the remarkable intrinsic properties of novel nanomaterials to render them capable of sensing specific biomolecules. Such miniaturized sensors could be integrated with automated lab-chip devices and deployed to diagnose molecular changes in biological systems and in diseases such as cancer (by targeting new cancer biomarkers) or to detect infectious agents in biological samples, e.g. in blood, saliva and urine. From a health industry perspective, we target the advancement of the automated and portable tools for in-field testing, remote locations and hospitals in close collaboration with clinicians to validate the devices with clinical samples. The proposed hybrid devices are capable of working with small sample volumes and precise dosing of reagents, enabling the transition to a portable diagnostic tool.

I106

ADVANCED ELEMENTAL ANALYSIS IN DIRECT LITHIUM EXTRACTION USING AGILENT ICP-OES.

Ana Garcia-Gonzalez, **Longbo Yang**. Agilent Technologies, 6705 Millcreek Drive, Mississauga, ON L5N 8B3, Canada. (longbo.yang@agilent.com)

Direct lithium extraction (DLE) is an emerging technology designed to efficiently and sustainably extract lithium from sources such as salt flats and geothermal fluids. Unlike traditional methods that rely on slow and resource-intensive evaporation ponds, DLE employs chemical processes, membranes or adsorbents to selectively and rapidly pull lithium from brines. To monitor and optimize the extraction process, DLE requires detailed elemental concentrations data at every stage. ICP-OES has become the industry standard for lithium brine analysis because of its ability to handle high salt content, perform multi-element determination and offer high sample throughput. However, specific analytical challenges are associated with lithium brines due to the high level of total dissolved solids (TDS), significant physical and chemical interferences, and varying analyte concentrations across different extraction stages. Addressing these challenges necessitates selecting the appropriate ICP instrumentation and sample introduction system. Agilent ICP-OES system provides a complete solution for lithium brine elemental characterization featuring robust hardware, smart software, automated workflow and optimized method. In this study, three typical types of brine samples from a commercial DLE process were measured for 12 key elements, demonstrating the robustness, efficiency, stability and accuracy of the Agilent ICP-OES solution.

I107

CONTINUOUS ON-LINE LEACHING BIO-ACCESSIBILITY STUDY OF MEALWORMS USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Qiqi Zhang**[1], Ellen Mcgivern, Diane Beauchemin[1], Zoltan Mester[2]. [1]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 2S8, Canada; [2]National Research Council of Canada, Metrology Research Centre, 1200 Montreal Rd, Ottawa, ON K1A 0R6, Canada. (17qz@queensu.ca)

Mealworm, as an environmentally sustainable food source, is considered a non-novel food according to Health Canada [1]. As no specific health or safety risks have been identified, they are not subject to safety assessment by Health Canada [1]. However, non-novel foods must still comply with all applicable food regulations [1]. As little is known about safe dosage/risk assessment that is normally determined based on total concentrations, an improved setup built upon the previously established continuous on-line leaching method coupled with inductively coupled plasma mass spectrometry (ICPMS) enabled the quick measurement of bio-accessible concentrations. The mealworm powder was loaded in a transparent polypropylene flash column and sequentially flushed with 37 °C artificial saliva and gastric juice while monitoring eluted elements by ICPMS. Mass balance was verified for As, Cr, Se, and Cd. Following the Guidance on Human Health Preliminary Quantitative Risk Assessment, individuals of all age groups (excluding infants) can safely consume mealworms at a level of 2.04×10^{-7}mg/kg bw/day.

[1] https://www.canada.ca/en/health-canada/services/food-nutrition/genetically-modified-foods-other-novel-foods/requesting-novelty-determination/list-non-novel-determinations.html

I108 P

QOLOREX FOR RAPID DEPLOYABLE MULTIPLEXED MOLECULAR TESTING. **Sahar S. Mahshid**, Beeta Biomed Inc., Clinical Innovation Platform, Montreal General Hospital, Montreal, QC, Canada. (sahar.mahshid@beetabiomed.com)

The detection of DNA and RNA as unique genetic markers is essential, particularly in infectious disease diagnostics, where rapid, accurate pathogen identification is critical to containment and treatment. Molecular diagnostics offers a robust method for identifying these genetic signatures, enabling precise disease detection and monitoring. Not too long ago, the world witnessed a viral infection that became the COVID-19 pandemic, as limited testing capacity contributed to unchecked spread. Today, the global community continues to face threats from high-risk pathogens like Marburg, Mpox, Avian Influenza, and Dengue. Several of these escalated into outbreaks in 2024, with the potential to become global health crises if left uncontrolled. Polymerase chain reaction (PCR) techniques remain the gold standard for molecular diagnostics due to their high accuracy. However, traditional PCR-based methods involve lengthy protocols, costly reagents, complex instruments, and require trained personnel. These demands drive the industry to seek alternatives that deliver multiplex results quickly—ideally within an hour—by minimizing time-intensive steps like sample preparation, nucleic acid extraction, and amplification. QolorEX is a user-friendly nucleic acid detection device using novel plasmonic nanostructures to provide colorimetric readouts with gold-standard accuracy for automated, deployable multiplex diagnostics. QolorEX is taking the journey toward commercialization while supported by McGill University and its dedicated research teams to drive progress in nucleic acid testing.

I109 P

HOW SAFE IS DRINKING WATER ON THE CAMPUS OF QUEEN'S UNIVERSITY?

Karissa Riopelle, Michael Trolio and Diane Beauchemin. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (diane.beauchemin@queensu.ca)

Safe drinking water is essential to public health, yet aging infrastructure can introduce harmful contaminants, including trace metals, into water systems. This study investigates the presence of trace elements in drinking water sources across Queen's University, a campus with buildings dating back to 1841. Several trace elements were determined, including Mn, Cr, Fe, Cu, Zn, As, Se, Cd, Sn, Hg, and Pb. These elements were selected for their known toxicological profiles and potential to bioaccumulate, with health effects ranging from nephrotoxicity and hepatotoxicity to neurotoxicity, carcinogenicity, and reproductive harm. The study aims to identify concentrations that exceed national and international regulatory limits, with particular attention to highly toxic metals such as Pb, Cd, Hg, and As, which are typically regulated at parts-per-billion levels. In contrast, Cu, Zn, and Fe have higher allowable thresholds. Sampling focused on high-use locations, including sinks, taps, and refill stations, with first-draw collection employed to reflect real-world exposure. Water samples were collected in the morning and in the afternoon in acid-washed containers, acidified with high-purity nitric acid to pH <2, and stored at 4 °C to preserve metal content. Quantification of trace elements was performed by inductively coupled plasma mass spectrometry using external calibration.

I110 P

COMPARISON OF INFRARED-HEATED SAMPLE INTRODUCTION SYSTEM WITH CONVENTIONAL ONE FOR CELL ANALYSIS BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY.

Xinzhi Cai, Zichao Zhou, Diane Beauchemin. Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (diane.beauchemin@queensu.ca)

Single cell inductively coupled plasma mass spectrometry (scICPMS) can detect and quantify elemental composition at the individual cell level, providing insights into cellular heterogeneity and trace element concentrations with high sensitivity [1]. However, conventional scICPMS typically suffers from low transport efficiency. To enhance analyte transport, an infrared (IR)-heated sample introduction system was employed [2]. This study compares the performance with an IR-heated sample introduction system versus a conventional one for scICPMS analysis. The Se-enriched yeast certified reference material SELM-1 was analyzed to ensure accuracy and reliability. The effects of IR heating temperature, spray chamber volume, sampling position, and sample uptake rate on sensitivity were studied. The integration of IR heating with optimized operational parameters significantly improves the performance of scICPMS for Se analysis, highlighting its applicability and potential impact in advanced trace element investigations within biological and environmental systems.

[1] J.S.F. Pereira et al., *Talanta*, 2022, **236**, 123786.
[2] Z. Zhou et al., *J. Anal. At. Spectrom.*, 2024, **39**, 2078–2086.

I111

STRUCTURAL BASIS OF GENE DEREGULATION BY THE DISORDERED TRANSCRIPTION FACTOR TCF3-PBX1 IN ACUTE LYMPHOBLASTIC LEUKEMIA – GUIDE TO PEPTIDE INHIBITOR DESIGN. David Langelaan, Marina Lochhead, Christopher Denis, Holly Spencer, David Lebrun, **Steven Smith**, Queen’s University, Department of Biomedical and Molecular Sciences, Kingston, ON K7L 3N6, Canada. (sps1@queensu.ca)

Disordered proteins play critical roles in numerous cellular functions, including transcription. The transcription factor TCF3 plays a fundamental and critical role in normal development of our immune cells from hematopoietic stem cells, a process class lymphopoiesis, However, a chromosomal translocation (1;19)(q23;p13) results in the expression of the chimeric transcription factor TCF3-PBX1 that is found in ~5% of B-cell precursor acute lymphoblastic leukemia (ALL) - cancerous hematological disorder originating in B-lymphoid progenitor cells. The oncogenic TCF3-PBX1 protein contains the transcriptional activation domains of TCF3 and most of the PBX1 protein, including the DNA-binding homeodomain. These structural features suggest a hypothetical model in which TCF3-PBX1 binds DNA, recruits transcriptional co-activators by means of the TCF3nactivation domains and induces ALL through deregulation of PBX1 target genes. This transcriptional control is, in part, mediated by the recruitment of the transcriptional coactivator CBP/p300. Indeed, previous studies have shown that TCF3-PBX1-mediated oncogenesis requires direct binding of TCF3-PBX1 to CBP/p300. In this presentation, we will describe our biophysical, structural, biochemical, genomics studies that have identified the genomic regions to which TCF3-PBX1 binds, have revealed the structural basis for the TCF3-PBX1:CBP/p300 interaction, and has allowed us to develop a novel molecular designer compound, which binds the KIX domain of CBP/p300 with high affinity and specificity, disrupts TCF3-PBX1:CBP/p300 complex formation, and downregulates TCF3-PBX1 target genes *in vivo*.

I112

DEVELOPMENT OF A CAPILLARY ELECTROPHORESIS ASSAY FOR Cu(I) AND Cu(II) TO ELUCIDATE THE COPPER LEACHING MECHANISM DURING PURIFICATION OF GRAPHITE FROM Li-ION BATTERY ANODE WASTE. **Karen C. Waldron**, Brunilda Rica and Mickael Dollé, Université de Montréal, Department of Chemistry, 1375 av. Thérèse-Lavoie-Roux, Montréal QC, H2V 0B3, Canada. (karen.waldron@umontreal.ca)

Recycling efforts for lithium ion batteries (LIBs) can be extended to include production scrap, a costly waste stream with respect to materials and delivery deadlines. Therefore, recycling electrode scrap is inevitable, including graphite from failed anodes. We recently developed a sustainable recycling approach based on aqueous organic acid leaching to purify graphite from failed industrial anodes, whose major impurity is copper from the current collector. During leaching, Cu(0) in the sample of sieved anode material (a black powder) is transformed by redox and chelation reactions to Cu(II) ions, thus easily removed from the purified graphite. We “presume” Cu^{2+} is the final product, based on the color of leachates after 60 min. Total copper in the solutions, ranging from 40 to 80 mg/L, was determined by AES, which provides no speciation information. To investigate the leaching mechanism, i.e., whether there is initial oxidation of Cu(0) to Cu(I), we are developing a capillary electrophoresis (CE) assay for copper speciation. CE requires very little sample, little or no sample prep, and is rapid. The goal is to interrogate leaching at various times to elucidate the redox processes. Capillary ion electrophoresis (CIE), i.e., CE for separation of inorganic and transition metal ions, often requires the use of chelating agents because of the highly similar mobilities, which are based on relative ionic conductance. Development of a rapid CIE method consisted of investigating complexing agents (EDTA, NTA, bicinchoninic acid, 1,10-phenanthroline) and indirect versus direct UV-Vis detection to reach quantitation limits of 10 mg/L, sufficient for determining Cu(I) and Cu(II). Results of the optimization and application to measurement in graphite purification leachates will be discussed.