I001

ANALYSIS OF CLAYS BY ICP-MS AND UNCONVENTIONAL APPROACH TO DATA INTERPRETATION**.** **Ela Bakowska** and Alind J. Barany Corning RDC, SP-DV-D2W69C, Corning, NY 14831, USA. (bakowskae@corning.com)

To determine the viability of ICP-MS as an analytical tool for determining the major elements of minute amounts in clays, we needed to develop an effective sample digestion method. Three different smectite clays were used for the method validation:

- Nontronite [$Na_{0.3}Fe_2(Si,Al)_4$ or $Ca_{0.5}(Si_7Al_{0.8}Fe_{0.2})(Fe_{3.5}Al_{0.4}Mg_{0.1})$],
- Montmorillonite $(Na,Ca)_{0.33}(Al,Mg)_2(Si_4)$,
- and synthetic Saponite $(Na,K)_{0.66}Mg_6(Si_{7.34}Al_{0.66})$,

The EPA 3052 method was insufficient to completely digest both Montmorillonite and Nontronite. A modified microwave digestion method using an acid combination of HCl, HNO_3, and HF resulted in complete dissolution of those clays. The resulting solutions were then analyzed by various analytical techniques. The sample preparation was then scaled down to smaller quantities of clay and the resulting solutions were analyzed by ICP-MS. The elemental concentration ratios were compared to the theoretical chemical compositions of different smectite clays. A cluster analysis of the elemental ratios was performed to successfully distinguish between the different clays.

I002

EXPLORING NEW ELECTRODES AND CHANNEL CELL DESIGNS FOR ELECTROANALYTICAL STUDIES UNDER HYDROTHERMAL CONDITIONS. **Liliana Trevani[1],** Muna Abdulaziz[1], Tony George[1], Germán Sciaini[2]**.** [1]Ontario Tech University, Faculty of Science, 2000 Simcoe St North, Oshawa (L1G 0C5), ON, Canada; [2]University of Waterloo, Department of Chemistry, 200 University Ave W, Waterloo (N2L3G1), ON, Canada. (liliana.trevani@ontariotechu.ca)

Electroanalytical methods have been extensively used for chemical analysis and mechanistic studies of complex redox processes for various applications.[1]. However, most techniques were developed for studies at relatively low temperatures and pressures (*T*,*p*). Electrochemical studies under hydrothermal conditions remain uncommon, mainly due to the need for relatively complex pressurized systems [2]. For analytical studies, high *T*,*p* flow cells, particularly channel flow cells (CFC), are advantageous for multisampling analysis and compatible with spectroscopic methods for operando studies [3]. In this presentation, I will describe a new high-temperature CFC design for electrochemical studies in pressurized aqueous systems and the problems found while constructing and evaluating the first prototype. Along with the cell, the project involved the development of Pt thin-film electrodes and numerical simulations that were used to gain insight into crucial cell parameters required for optimizing the system. These aspects will also be discussed in the presentation.

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[3] H. Wang, E. Rus, H. Abruña, Anal. Chem. 2010, 82:4319-24.

I003

VITAMIN B_{12} DETERMINATION IN NUTRITIONAL PRODUCTS AND DIETRAY SUPPLEMENTS BY HPLC-ICP-MS. **Mesay M. Wolle**,[1] Jordan Escavage[2] and Patrick Gray[1] [1]Office of Regulatory Science, Center for Food Safety and Applied Nutrition, Food and Drug Administration, 5001 Campus Drive, College Park, MD 20740, USA; [2]Joint Institute for Food Safety and Applied Nutrition (JIFSAN), University of Maryland, College Park, MD 20742, USA.

Vitamin B_{12}, also known as cobalamin, plays a key role in red blood cell formation and functioning of the brain and nervous system. Cobalamins are only found in animal products such as meat, eggs, and dairy but B_{12} intake can be increased by consumption of dietary supplements and fortified foods. Accurate quantification of the distinct forms of vitamin B_{12} (i.e., cyano-, hydroxo-, adenosyl- and methyl-cobalamin) is important because of the differences in their metabolism. Historically used B_{12} methods such as microbiological assays, radioisotopic analysis, and spectrophotometry are limited in sensitivity, specificity between forms of B_{12}, and/or efficiency. In this presentation, a method development and single-lab validation study that provides for specific, accurate and reliable measurement of vitamin B_{12} in products including infant, pediatric and adult formulas, protein drinks, milk, and breakfast cereals will be discussed. The methods are based on liquid extraction followed by analysis using high performance liquid chromatography interfaced with inductively coupled plasma-mass spectrometry (HPLC-ICP-MS). Single-lab validation of method and comparison with AOAC Official Method 2014.02, and microbiological assay will be covered.

I004

SELF-ASSEMBLING MONOLAYERS OF LATE TRANSITION COMPLEXES FOR ULTRA-STABLE ELECTROCHROMIC MATERIALS AND DEVICES. Rana Ahmad, Vittoria Di-Palo, E. Bradley Easton, **Olena V. Zenkina.** Ontario Tech. University, 2000 Simcoe Street North, Oshawa, Ontario, Canada. (Olena.zenkina@ontariotechu.ca)

Covalent attachment of the well-defined transition metal adducts of terpyridines into high surface area screen-printed electrodes is a powerful strategy to access durable electrochromic materials with great long-term durability, high colour contrast and fast switching speeds. Here we demonstrated how tuning of molecular structures in solution before the deposition or on-surface post-modification approach could be utilized to tune the colours of the electrochromic monolayers. In addition, we explored the energy storage potential of the hybrid electrochromic devices and explored the role of the counter electrodes on device degradation pathways. We studied the role of various components of the electrochromic devices in the overall stability of the devices and systematically optimized their performance in terms of operation potential window and long-term electrochemical durability; explored the nature of the processes on the interface between the electrochromic working electrode, gel electrolyte and counter electrode. Finally, we developed novel double-side device configurations that could operate in unilateral and bilateral modes and demonstrate unprecedented durability of 10^5+ electrochemical cycles [1].

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I005

CONJUGATED POLYMER NANOPARTICLES AS A UNIVERSAL HIGH-AFFINITY PROBE FOR THE SELECTIVE DETECTION OF MICROPLASTICS IN THE ENVIRONMENT. **Mark Potter**, Angela Awada, Dananjana Wijerathne, James W. Gauld, Bulent

Mutus, and Simon Rondeau-Gagné. Department of Chemistry & Biochemistry, University of Windsor, 401 Sunset Avenue, Windsor, ON N9B 3P4, Canada.

Microplastic (MP) contamination has become one of the major environmental concerns of the 21st century. MPs are formed by the natural degradation of plastic-waste, and with less than 9% of the ~6.3 billion tons of cumulative plastic waste being recycled; the number of environmental MPs is steadily increasing. Current MP-identification and detection methods can be time-consuming due their heavy reliance on laborious, complex extraction, and concentration steps. As a result, very little is known about MPs with respects to their environmental or biological impact. In this presentation, we will discuss a novel design for the selective detection of MPs by exploiting fluorescent conjugated polymer nanoparticles (CPNs). The affinity of the CPNs and their components to various MPs were explored via fluorescent microscopy, and computational studies. A very strong affinity to a broad range of MPs was observed with apparent dissociation constant ($K_{D,App}$) values in the picomolar range. These CPNs were shown to be selective to MPs even in the presences of soil debris and other organic contamination. In addition, we will discuss the ability to use these CPNs with a variety of environmental samples, enabling the fluorescence-based detection of MP contaminants irrespective of their origins, collection techniques, or structural characteristics.

I006

LASER-INDUCED BREAKDOWN SPECTROSCOPY FOR THE DETECTION AND DIAGNOSIS OF BACTERIAL PATHOGENS IN BLOOD, URINE, AND CEREBROSPINAL FLUID.

Emma Blanchette[1], Emily Tracey[1], Caroline Alionte[1], Hadia Malik[1], August Baughan[1], Isabella Arthur[2], Jasmine Saad[1], Rachel Chevalier[2], Nicholas Bolton[1], Matteo Pontoni[1], Lauren Dmytrow[1], Abdullah Mustafa[1], Mila Vasquez[1], and **Steven J. Rehse**[1]. University of Windsor, [1]Department of Physics and [2]Department of Biomedical Sciences, Windsor, ON, Canada. (rehse@uwindsor.ca)

In this work, laser-induced breakdown spectroscopy, or LIBS, has been utilized to detect and diagnose common bacterial pathogens in clinically obtained specimens of whole blood, urine, and artificial cerebrospinal fluid (aCSF). A custom-fabricated centrifuge insert allowed bacteria to be easily collected from a fluid specimen and concentrated at the center of a disposable nitrocellulose filter prior to LIBS testing. The measured intensities of emission lines from five elements were used as independent variables in a partial least squares discriminant analysis to classify specimens as either bacteria-negative or bacteria-positive, achieving sensitivities and specificities greater than 96%. A diagnosis of the species of bacteria present in the specimens was accomplished by performing a principal component analysis on the entire LIBS spectrum from 200 nm to 590 nm. The first 10 principal component scores from that analysis were used as independent variables in a single hidden layer artificial neural network analysis, resulting in classification accuracies in excess of 80%. These results indicate the potential usefulness of LIBS for rapidly detecting and possibly diagnosing blood infections (sepsis), urinary tract infections, and bacterial meningitis in a clinical setting.

I007

ENVIRONMENTAL CHEMISTRY: CHALLENGES AND POSSIBLE IMPACT OF ELEMENTS AND SMALLEST PARTICLES.

Petra Krystek, Deltares, Utrecht, The Netherlands. (petra.krystek@deltares.nl)

Especially in the last decade, the energy transition towards renewable energies and sustainable processes is growing enormously. Currently, renewable energy resources by solar and wind are dominating. Having a closer look to the materials used in renewable energy technologies, then especially metals and elements as well as the so-called ‘technology critical elements' stand out. Within case studies, photovoltaic solar materials were investigated more closely under various environmental circumstances. New insights were gathered by time-dependent leaching experiments followed by inductively coupled plasma mass spectrometry (ICP-MS) analysis. For the total materials characterization, a non-destructive technique like instrumental neutron instrumental neutron activation analysis has advantages. Challenges in the methodological set-up like possible contaminations and the toxicity of the related elements and metals will be discussed. In environmental analysis, progressive approaches are needed for studying emerging contaminants, such as engineered, inorganic nanomaterials. By linking ICP-MS research, bottlenecks are often the related validations of complete methods and quality criteria while aspects like reliability and reproducibility become more relevant. Workflows often start with sample pretreatments in the laboratory followed by instrumental analysis for the identification and/or detection of nanoparticles. Especially for the ultra-trace analysis of nanomaterials in environmental matrices, the sampling is of the utmost importance in analytical workflows. The sampling is often underexposed and possible errors at these steps influence the validity of final results. Within this presentation, a special focus will be laid on sampling strategies of nanoparticle analysis for various types of water samples in the complete water cycle.

I008

INFLUENCE OF ANTICOAGULANT ON THE SPECTROSCOPIC ANALYSIS OF DRYING BLOOD POOLS.

Erin Giroux[1], Iraklii I. Ebralidze[2,3], Theresa Stotesbury[1,3], [1]Applied Bioscience Graduate Program, [2]Materials Characterization Facility, [3]Faculty of Science, Ontario Tech University, 2000 Simcoe St N, Oshawa, ON L1G 0C5, Canada. (erin.giroux@ontariotechu.net)

In minutes, untreated whole blood undergoes a clotting cascade making forensic research that investigates “fresh” bloodletting events difficult. In bloodstain pattern analysis research, whole blood treated with anticoagulant is often used to prolong the blood’s “shelf-life” and experimental useability for realistic forensic simulation. Here, we investigate the spectral implications of anticoagulant addition for time since deposition (TSD) estimation methods of larger volume blood pools. Differences in spectral profiles of blood pools with and without a citrate-based anticoagulant were characterized using visible absorbance spectroscopy, Attenuated Total Reflection-Fourier Transform Infrared (ATR-FTIR) spectroscopy, and X-ray Photoelectron Spectroscopy (XPS). Across all methods, notable spectral differences were observed between treated and untreated blood pools. Principal Component Analysis was used to further assess these differences in the visible absorbance and ATR-FTIR spectra over time. The blood pools differed most significantly ($p<0.0001$) in the first week following deposition due to the slowed drying of blood pools treated with ACD-A, whereas at timepoints exceeding one week following deposition, the spectral profiles of the pools regained similarity. These findings are consistent with physical drying TSD methods. Thus, the inclusion of anticoagulant is an important consideration during experimental design and analysis for both physical and spectral TSD estimation methods.

I009

ION CONDUCTING MEMBRANES FOR CLEAN ENERGY SYSTEMS.

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Chemical Engineering, Toronto Metropolitan University, Toronto, ON M5B 2K3, Canada (jkaur2@brocku.ca)

Ion conducting membranes have been employed as electrolytes in clean energy conversion, and storage systems, such as water electrolyzers, supercapacitors and batteries. These electrolytes serve as one of the core components and directly determine the performance and durability of electrochemical devices. However, the traditional proton exchange membranes and anion exchange membranes suffer from highly toxic preparation procedures, poor chemical, and electrochemical stabilities, and low ionic conductivities. This has initiated scientists to explore alternative inorganic building blocks and innovate novel material designs for improving the performance and stability of devices. The recently growing research on two-dimensional (2D) materials has shown exceptional properties, including high ionic conductivities, which enhances the feasibility of fabricating high performance 2D material-based electrolytes. In this work, we have created superionic solid-state electrolytes by nanoengineering the surface of 2D material, hexagonal boron nitrides (h-BN) and integrating them in polymer structure to cast specific ion conducting membranes. 2D h-BN nanoflakes and the developed electrolytes are characterized by advanced spectroscopic and microscopic techniques, including electrochemical impedance spectroscopy. The 2D h-BN electrolytes turn out to be highly conductive, electrochemically stable, and mechanically robust, allowing selective ion conduction for various types of ions, including protons, hydroxides, and lithium ions.

I010

HIGHLY SENSITIVE MULTIPLEXED PROTEIN ANALYSIS IN PLASMA AND EXTRACELLULAR VESICLES. Rebecca Goodrum, **Huiyan Li**, School of Engineering, University of Guelph, Canada. (huiyanli@uoguelph.ca)

Proteins are the nanomachines in the body that function in various biological processes. Quantifying protein concentrations in complex biological samples such as plasma and extracellular vesicles can provide important information on health and diseases [1]. Conventional methods, such as enzyme-linked immunosorbent assay (ELISA) is a sensitive and reliable approach for protein quantification, but has limited analytical sensitivity and multiplexing capability that cannot meet clinical needs for early diagnosis of some complex diseases such as cancer. Other methods such as conventional mass spectrometry and western blotting have limited sensitivity, and sometimes are semi-quantitative [2]. In this talk, I will present several new biosensing platforms that we have recently developed. These platforms have been applied for protein quantification in plasma, cells, and extracellular vesicles, and have achieved higher assay sensitivity by a few orders of magnitude compared to those of conventional assays. The high sensitivity, multiplexing capability, and ease of use makes these new biosensing platforms suitable for a variety of applications in biological and biomedical research, such as early cancer diagnostics and biomarker discovery.

[1] A. Bodaghi, N. Fattahi, A. Ramazani. Heliyon. 2023. E13323.
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I011

X-RAY PHOTOELECTRON SPECTROSCOPY (XPS) FOR IN-DEPTH STUDY OF METAL COMPLEXES. **Iraklii I. Ebralidze**, E. Bradley Easton. Ontario Tech. University, Faculty of

Science, Materials Characterization Facility. 2000 Simcoe Street North, Oshawa, ON, L1G 0C5, Canada. (Iraklii.Ebralidze@ontariotechu.ca)

The progress made recently in material science and forensics is largely attributed to the advancement of instrumental techniques that enable the analysis of matter at the nanoscale. X-ray photoelectron spectroscopy (XPS) is a powerful surface analytical tool that allows accurate determination of ligand-to-metal ratios, oxidation states of metals, and even the thickness of layers formed on the surface. Non-destructive nature of XPS analysis enables obtaining high-quality data without affecting the integrity of the specimen, which makes XPS a valuable tool for both academia and industry. We will discuss the utilization of XPS for the analysis of ligands and organometallic compounds deposited on appropriate supports for the design of mono- and multilayer-based materials, as well as for the synthesis of metal nanoparticles. The applications of these materials are very broad and include detecting and removing heavy metals, developing electrochromic materials and supercapacitors, etc. In addition, we will touch upon the possibility of using XPS in forensic science to analyze the degradation of blood pools. Based on the examples provided, you will see that the insights gained from XPS analysis of metal complexes have the potential to drive innovations in diverse fields, from water quality and sustainable energy technologies to forensic science.

I012

SPECIATION OF NITROGENOUS-COMPOUNDS WITH P-TOLUENESULFONYL CHLORIDE DERIVATIZATION FOLLOWED BY LC-MS. **Ran Zhao**, Xinyang Guo, Kimberly Wong, Department of Chemistry, University of Alberta, Canada. (rz@ualberta.ca)

Nitrogenous compounds, including ammonia, amines, and amides, play an important role in a wide variety of environmental and biological progresses. Detection of small nitrogenous compounds in environmental samples is challenging. These compounds can have high polarity, low ionization efficiencies with common mass spectrometry (MS) ion sources and are usually found in complex environmental matrixes. Derivatization with p-toluenesulfonyl chloride (TsCl) is known to be selective to amino-nitrogenous compounds and has been previously used in the detection of amines in beverages. In this presentation, I will showcase two applications of this derivatization method to environmental samples. Combined with liquid chromatography (LC)-MS, our method achieved excellent selectivity and sensitivity towards amines and amides that are of great environmental importance. In the first application, my team detected and quantified key species, such as uric acid and dimethylamine, in a commercial poultry facility. These compounds are precursors to ammonia, a toxic gas often cumulated in indoor poultry facilities. In the second application, we characterized oxidation products of nicotine in e-cigarette juices (e-juices). This study shows that e-juices can be slowly oxidized during storage, with their nicotine contents forming unrecognized and potentially harmful nitrogenous products.

I013

LOCALIZED SURFACE PLASMON RESONANCE SPECTROSCOPY: APTAMER AND PROTEIN INTERACTIONS. **Tyra Lewis**[1], Erin Giroux[1], Amanada Oake[2], Sanela Martic[1]. [1]Department of Forensic Science, Environmental and Life Sciences, Material Sciences Program, Trent University, Peterborough, ON, Canada. [2]Flemming College, Peterborough, ON, Canada (sanelamartic@trentu.ca)

The SARS-CoV-2 spike (S) glycoproteins are known to bind to the angiotensin converting enzyme 2 (ACE2) receptor to initiate a viral infection. Hence, the S protein plays an important role in the function of the virus and can be useful diagnostic biomarkers.1 Moreover, the S-ACE2 binding interface is also a promising target for anti-viral therapeutic strategies. Short single-stranded nucleic acid sequences known as aptamers, provide a highly specific affinity to targets, and minimal cross-reactivity.1 Due to strong binding properties, they are used in biosensors as effective binding partners toward targets such as proteins. Additionally, they can act as inhibitors to prevent viral infections, whereby the aptamer serves as a blocker of virus-host interactions, such as SACE2.1 Heparin is also a known binder of SARS-CoV-2 S protein. Herein, we demonstrate the use of localized surface plasmon resonance (LSPR) as a technique for monitoring aptamer and heparin interactions with SARS-CoV-2 S protein, as well as their inhibition of S-ACE2 binding.2,3 LSPR binding data and molecular docking simulations were used to determine binding affinity and evaluate the aptamer-protein interactions, protein-protein interactions and S-ACE2 inhibition. The S aptamer showed universal binding to the SARS-CoV-2 wildtype or mutant S proteins and inhibited all S-ACE2 complexes to varying extents. Heparin was effective against all mutantACE2 complexes. Notably, factors such as steric hindrance near the binding site and conformational changes of the S protein can affect inhibitory behavior. Overall, data indicate that LSPR is a viable tool for measuring SARS-CoV-2 related aptamer-protein and protein-protein interactions.

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I014

RCMP TRACE EVIDENCE SERVICES: WHAT WE DO, WHAT WE DON’T. **Claude Dalpé**, RCMP-GRC National Forensic Laboratory Services, NPS Building, 73 Leikin Drive, Ottawa, ON K1A 0R2, Canada. (claude.dalpe@rcmp-grc.gc.ca)

In this presentation we are going to expose the Big Picture of the different forensic services offered by the National Forensic Laboratory Services at the Royal Canadian Mounted Police with a focus on Trace Evidence Services (/chemistry). An overview of Trace Evidence Services personnel competency requirements will be presented including the laboratory locations in Canada with their different forensic services offered. Some exhibits selection/criteria for Trace Evidence Services will be discussed with the emphasis on “what we accept” and “what we don’t accept”. Each service will be covered in term of their forensic limitation and their outcomes for court intention. At the end a quick overview of ongoing Research and Development will be presented with future direction.

I015

PROBING ELECTROCHROMIC DEVICE STABILITY USING ELECTROCHEMICAL IMPEDANCE SPECTROSCOPY.Rana Ahmad, Vittoria Di-Palo, Marjan Saeidi, Olena V. Zenkina, **E. Bradley Easton,** Ontario Tech. University, 2000 Simcoe Street North, Oshawa, Ontario, Canada. (brad.easton@ontariotechu.ca)

Electrochromic (EC) materials are a class of "smart" materials that change their optical properties in response to an applied potential. We have developed an EC system that contain as little as a monolayer of the EC molecules deposited onto a surface-enhanced conductive support. The process involves the covalent attachment of various ligands to the surface of a conductive indium − tin oxide (ITO) nanoparticles support. Subsequent reaction with metal ions (e.g. Fe, Ru) leads to the formation of a monolayer of the redox-active metal complex that is covalently bound to the ITO support. Our fabrication approach relies upon the inter-particle porosity of the support and requires as low as a monolayer of EC active molecule, giving significant molecular economy compared with traditional polymer-based EC devices. Despite the growing popularity of these devices, the understanding of the factors that influence their electrochemical performance and stability is still in its infancy. Better electrochemical diagnostic methods are needed to understand the modes of degradation. This presentation will focus on how detailed electrochemical studies that employ electrochemical impedance spectroscopy (EIS) can be used to determine the device degradation pathways. Based on this, improved EC device designs are proposed and validated.

I016

BIOELECTROCHEMISTRY: WHAT CAN WE LEARN ABOUT BRAIN PROTEINS **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.

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I017

TRANSFER AND PERSISTENCE ANALYSIS OF GUNSHOT RESIDUE BY MP-AES AND ICP-MS. Deanna Haas[1], Shannon Accettone[1,2], David Ruddell[3], **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) involves the deposition of metal particles emitted from a firearm [1]. The combination of lead, barium, and antimony is characteristic of GSR particles. Among the challenges in using this evidence is the transfer and persistence of these particles. Specifically, the transfer and persistence of GSR on fabrics are of forensic relevance (primary, secondary or tertiary transfers). The detection and quantification at these trace metal levels are required for evidentiary analysis of gun-related crimes [2]. Herein, metal transfer and persistence on fabrics were evaluated using MP-AES and ICP-MS instruments. Various GSR-contaminated fabrics were analyzed for intra-transfer and intertransfer of GSR. GSR transfer during evidence packaging was probed. Metal deposition heat maps were generated to monitor GSR location on the fabrics. All metals were found during transfer studies, but the amount of transfer was highly dependent on the fabric type. Data provide additional insight into the GSR transfer and persistence which is of value to forensic scientists.

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[2] M Christopher et al. Analyst (2013) 4649-4655.

I018

CHARACTERIZING THE SPATIO-TEMPORAL VARIABILITY OF DISSOLVED ORGANIC MATTER MOLECULAR COMPOSITION AND METAL TRANSPORT IN AN AGRICUTRUALLY IMPACTED WATERSHED. **Mary Chris Lagumen**, Lisa Harris, Taryn Petrovsky, Aaron Kizel, Vaughn Mangal Department of Chemistry, Brock University, St. Catharines, ON, Canada. (uu22sv@brocku.ca)

Land disturbance in the form of agriculture changes the natural biogeochemical cycling of many contaminants and organic carbon. Identifying how water quality is spatially and temporally varies within an agriculturally impacted watershed is important to better understand how changing water quality within aquatic ecosystems. In this study, we sampled water (groundwater, surface, rain, and porewater), soils, and sediments from 5 different sites along the Wignell Drain in the spring and summer of 2023 to highlight relationships between metal concentrations, organic carbon concentration and composition. Using water isotope information and Fourier Transform Ion Cyclotron Resonance Mass Spectroscopy (FT-ICR-MS), we found that stream water in the spring was characterized as predominantly groundwater and shifted to more surface runoff towards the later sampling dates (May to October) coinciding with the presence of aliphatic compounds (high H/C) that diminished towards the later sampling dates as surface runoff increased. Higher dissolved metal concentrations were also related to greater dissolved organic matter (DOM) molecular diversity, suggesting that a combination of hydrology and disturbance shape DOM-metal co-transport from soils and sediments in agriculturally disturbed watersheds.

I019 P

EXPLORING THE CHEMICAL COMPOSITION OF AEROSOLIZED eLIQUID THROUGHOUT THE LIFETIME OF ELECTRONIC NICOTINE DELIVERY SYSTEMS.

Tyra Lewis[1], Mehdi El Hassani[2], Olivier Bourbonnais[2], Christelle Luce[2], Sanela Martic[1]. [1]Department of Forensic Science, Environmental and Life Sciences, Material Sciences Program, Trent University, Peterborough, ON, Canada, [2]Ditch Labs, Montreal, QC, Canada. (sanelamartic@trentu.ca)

Electronic nicotine delivery systems (ENDS) were introduced as a healthier option to traditional cigarettes, however concerns about their safety remain.1 By comparison, ENDS produce a nicotine containing aerosol rather than generating a flame or smoke, and therefore reduces the user's exposure to tobacco smoke related toxicants [1,2]. The components of ENDS include a metal heating element and liquid-containing cartridge that consists of propylene glycol (PG) and/or glycerin (GLY), flavorings, organic acid, and nicotine as the main ingredients [2]. As the ENDS device is used, undesired and harmful carbonyls and aldehydes can be generated due to thermal decomposition of PG and GLY [2]. Exposure to these compounds can contribute to cardiovascular illness and lung related complications [1]. Additionally, coil deterioration with continued usage can lead to decreased efficiency for nicotine delivery, and unwanted leaching of components into the eLiquid [2]. Herein, the composition of organic and inorganic products in aerosols generated from eLiquid pods were explored, as a function of ePod usage. Gas chromatography-mass spectrometry (GC-MS) and inductively coupled plasma-mass spectrometry (ICP-MS) were used to identify and quantify the decomposition products or metals in the captured aerosol, respectively. Data suggests gradual changes to the concentrations of ingredients in the eLiquid throughout the lifetime of the pod, and significant levels of metal. Overall, this research provides valuable insights into the chemistry related to ENDS, which may inform consumers, industry, and government.

[1] Uchiyama, S., et al. Anal. Sci. (2016), 32:549–555.
[2] Saleh Q.M., et al. Int. J. Environ. Res. Public Health, (2021), 18:4380.

I020

RAPID, EFFICEINT MICROWAVE-ASSISTED DIGESTION OF PLANT-BASED MILKS FOR TRACE METALS ANALYSIS.

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Plant-based milks are becoming increasingly popular alternatives to dairy milk. While some plant-based milks, such as soy and almond, have become mainstream, more and more alternative milks, such as coconut and oat milk are also increasing in popularity. These non-dairy milks are derived from nuts, seeds, and other plant-based sources. Many plants and nut trees are effective bioaccumulators of inorganic compounds. Plants uptake metals from soils via the root and vascular system and can concentrate elements in the leaf, fruit, and flower. As these plants are processed into downstream products (such as non-dairy milks), plants grown in contaminated soil can accumulate heavy metals, increasing a consumer's heavy metal exposure. The heavy metals known as the big four (As, Pb, Cd, Hg) are of particular concern due to their potential toxicity. In this study, metal concentrations are measured and compared for plant-based milks and cow's milk. The metals are measured after microwave digestion and ICP-MS analysis of the milks.

I021

FLUORINE AND FLUORINATED COMPOUNDS – METHODS FOR DETERMINATION (OVERVIEW). **Andrea Raab** and TESLA (trace element speciation lab Graz), University of Graz, Austria. (andrea.raab@uni-graz.at)

Fluorinated compounds, often called forever chemicals, are nowadays talked about everywhere. The major reasons for this are their widespread use, their environmental persistence and their known or suspected health effects. From an analytical point of view these compounds present several challenges. For one this group is highly diverse. It ranges from molecules containing only one fluorine to fully fluorinate compounds. For known ionisable compounds with available standards LC-ESI-MS/MS is a suitable technique often reaching the required sensitivity. For unknown compounds or such that do not ionise in ESI determination is a significant problem. Tackling the problem from the elemental side using fluorine detection is not easy either. The techniques for detecting fluorine are not yet well established and not very sensitive. Fluoride can be detected using either a fluoride sensitive electrode or a conductivity detector combined with an anion exchange LC. The determination of organo-fluorines is not possible with these techniques. Combustion ion chromatography (CIC), molecular absorption spectrometry (CS-MAS) and ICPMS/MS allow the detection of fluoride and organo-fluorine compounds. The latter also in combination with separation methods. All these “elemental” methods still lack sensitivity and to some extent at least reliability. In the presentation some of these techniques, their possibilities in actual applications and their associated problems will be shown.

I022

DEVELOPING MULTIPLEXED ELECTROCHEMICAL DETECTION METHODS FOR MONITORING MANGANESE (Mn) 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 can have negative neurological effects on children. Although there are effective drinking water treatment processes to remove Mn, trace levels leaving the treatment plant can accumulate on distribution system pipe materials, forming a reservoir. Through shifts in chemical, hydraulic and microbiological stability, Mn reservoirs can be released back into bulk drinking water and arrive at consumers taps at levels exceeding the health-based maximum allowable concentration. Current traditional spectroscopic techniques for the detection of Mn are highly sensitive; however, they cannot be readily applied for real-time monitoring in distribution systems due to their size, cost, and operational requirements. Recently, electrochemical methods have been explored as portable, low-cost options; however, they face detection difficulties due to the complexity of a drinking water matrix. Thus, there is critical need for the development of a real-time monitoring tool for Mn in drinking water. In this research, a multichannel detection method using chronoamperometry is explored for its ability to detect Mn^{2+} in the presence of common drinking water interferents using pattern recognition. These generated patterns are analyte and concentration dependent and could be used to identify Mn^{2+} in real drinking water samples.

I023

INTRODUCING OXYGEN-17 LABELS ONTO L-THREONINE SIDECHAIN. **Yuying Huang** and Gang Wu. Department of Chemistry, Queen’s University, 90 Bader Lane, Kingston, Ontario, Canada K7L 3N6. (17yh99@queensu.ca)

Nuclear magnetic resonance (NMR) is a powerful spectroscopic tool that permits chemists to obtain detailed information about molecular structures. The most commonly used NMR-active nuclei are ^{1}H, ^{13}C, ^{15}N, and ^{31}P, all of which have $I = 1/2$. While the presence of oxygen element in many organic and biological molecules makes it a potential NMR target, the only NMR-active oxygen isotope, ^{17}O, is not only quadrupolar ($I = 5/2$), but has a very low natural abundance (0.037%). Both of these factors make ^{17}O NMR studies challenging [1]. The first step in many ^{17}O NMR studies is to introduce the ^{17}O isotope into the targeted functional group in the molecule of interest (i.e., ^{17}O-isotope labeling). It is well established that ^{17}O-isotope labeling of the carboxylate group in amino acids can be readily achieved [1]. However, ^{17}O-isotope labeling of the hydroxyl group in amino acid sidechains such as L-serine and L-threonine has remained a challenge. The sidechain hydroxyl group in proteins is known to play indispensable roles in many cellular processes. In this presentation, we report a convenient synthesis of [[3-^{17}O]-L-threonine where the sidechain hydroxyl groups are ^{17}O-labeled.

[1] G. Wu, Prog. Nucl. Mag. Reson. Spectrosc. 52, 118-169 (2008).

I024

SEQUESTERING POLONIUM FROM COPPER USING RESIN-BOUND CROWN ETHER. **Heather M^{c}Callum**[1,2], Emily Corcoran[2], Fiona Kelly[2], Zhe She[1]. [1]Queen’s University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. [2]Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 13 General Crerar Crescent, Kingston, ON K7K 7B4. (23QN21@queensu.ca)

Weakly interactive massive particles (WIMPs) are favoured candidates for dark matter. However, their rare interaction with conventional matter renders detection challenging. The NEWS-G collaboration has developed a WIMP detector utilizing a 140 cm, 99.99% pure copper sphere within archaeological lead and high-density polyethylene. Exposure to Rn-222 during sphere production and transportation may have caused contamination. Consideration of daughter radionuclides indicates that Pb-210 and Po-210, represent the most important background contributors. As a source of αdecay, reduction of Po-210 is a priority. Although, polonium has a favourable standard electrode potential, its low concentration favours preferential rereduction in the presence of copper metal. Thus, a polonium sequestrant has been used to kinetically remove polonium from its solution-metal surface equilibrium. Resin-bound 4,4′(5′)-di-t-butylcyclohexano 18-crown-6 crown ether displays a high affinity for polonium(IV) at low pH. Replicate experiments have studied artificially contaminated copper surfaces at Po-209 activities of *ca.* 1 Bq/cm^{2}, a factor of 10^{5} greater then in the detector. It is evident that oxidative acidic etching liberates polonium from copper surfaces and, that use of resin at solution loading of *ca.* 0.1 g/cm^{3} provides > 80% Po-209 sequestration. Ongoing studies are progressively reducing Po-209 contamination to determine the relationship between activity and sequestration efficiency.

I025

DETECTION OF *ESCHERICHIA COLI* AND ANTIBIOTIC-RESISTANT BACTERIA BY MONITORING BIOMOLECULES USING ELECTROCHEMISTRY; **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). In 2019, the CDC reported more than 2.8 million infections and 35,000 deaths caused by antibiotic-resistant bacteria and fungi in the USA alone. Current methods for detecting bacteria and ARB rely on culturing in lab facilities, use analytical instrumentation with trained personnel, and can take up to 48 hours or more to obtain results. These methods cannot be used for rapid, routine testing of ARB nor for on-site real-time monitoring, especially in remote areas. The ability to detect and monitor ARB contributes to understanding and characterizing antimicrobial resistance and can inform policy.

The recent SARS-CoV-2 pandemic demonstrated the efficiency and accessibility of point-of-care and self testing. This research addresses the demand for rapid, low-cost, portable, sensitive, and specific detection of ARB. Electrochemical (bio)sensors can detect bacteria and ARB directly, such as by antibody binding, or indirectly as demonstrated effectively in this work with the successful detection of *Escherichia coli* by monitoring 4-methylumbelliferyl-β-D-glucuronide hydrolysis by β-glucuronidase. The versatility of (bio)sensor designs presents an opportunity to develop a multiplexed electrochemical (bio)sensor device for multiple bacterial and ARB analytes.

I026

ELECTROCHEMICAL DETECTION OF SILVER NANOPARTICLES IN FRESHWATER: DEVELOPMENT OF A HIGHLY SENSITIVE METHOD. **Saheda Tamanna**[a], Zhe She[a], Louise Meunier[b] [a]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; [b]Queen's University, Department of Chemical Engineering, 19 Division St, Kingston, ON K7L 3N6, Canada. (22kd24@queensu.ca)

Silver nanoparticles (AgNPs) are showing up in many applications across medicine and industry because of their unique properties, including antibacterial and catalytic activity. However, the growing use of AgNPs results in inevitable environmental release and their essentially unknown impact on human health and ecosystem. The toxicity of AgNPs varies with concentration, size, shape, and surface charge. Yet, detecting AgNPs requires complex analytical processes. This research aims to develop a portable, sensitive, and cost-efficient electrochemical sensing method to detect AgNPs in freshwater systems. In a first step, AgNPs redox behavior from silver complexes was characterized by cyclic voltammetry (CV). This provided insights into how AgNPs undergo oxidation (loss of electrons) and reduction (gain of electrons) reactions during the voltage sweep. Secondly, to enhance the sensitivity and selectivity for AgNPs, graphene-nanocomposites were integrated onto the surface of glassy carbon electrode (GCE) by drop-casting. CV was used to characterize the redox behavior of AgNPs on bare GCE, and graphene-nanocomposite modified GCE. AgNPs showed higher oxidation current responsiveness on graphene-nanocomposites modified GCE compared to bare GCE because of excellent conductivity and large available surface area of graphene. These results indicate that graphene-nanocomposites may be a suitable sensing platform for AgNPs in environmental analysis.

I027

MERCURY DYNAMICS IN CONTAMINATED RIVER SYSTEMS AND THERMOKARST LAKES. **Holger Hintelmann**, Trent University, Peterborough, Canada. (hhintelmann@trentu.ca)

Atmospheric deposition of Hg may have decreased over most of Canada. However, Arctic envrionments are believed to store large quantities of both mercury and organic carbon, which are potentially released during periods of global warming. Especially the mobilization of mercury and its export to arctic aquatic ecosystems may pose as serious threat to both wildlife and northern communities living off the land. Another concern is the bacterial formation of methylmercury (MMHg), which could be elevated in thermokarst lakes.

This presentation describes the application of mercury isotope tracers and isotope ratio measurements to characterize sources of Hg in the Mackenzie River Basin (MRB) and the formation of methylmercury in several thermokarst lakes in Nunavik. We found that particulate Hg in the MRB is mostly associated with terrestrial sources, while the dissolve Hg fraction in river water is linked with present-day organic carbon and most likely originates from atmospheric deposition. The water column of investigated thermokarst lakes had higher THg concentrations in winter with a very high average proportion of 80% MMHg. In the summer, THg and the proportion of MMHg dropped. In sediments, Hg concentrations were less variable in both seasons. Results further showed high Hg methylation potential in both seasons.

I028

DUAL PORT CHAMBER FOR ICP-MS IN RADIONUCLIDE ANALYSIS. **Kayo Yanagisawa**[1,2], Makoto Matsueda[2,3], Makoto Furukawa[2,4] and Yoshitaka Takagai[2] (1) Japan Atomic Energy Agency, Nuclear Science and Engineering Center, Research Group for Nuclear Chemistry, 2-4 Shirakata, Tokai, Ibaraki 319-1195, Japan. (2) Fukushima University, Cluster of Science and Technology, 1 Kanayagawa, Fukushima 960-1296, 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., 134 Godo, Hodogaya, Yokohama, Kanagawa 240-0005, Japan. (yanagisawa.kayo@jaea.go.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. Inductively coupled plasma mass spectrometry (ICP-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 a dual-port cyclonic spray chamber with a concentric nebulizer and gas port. The spray chamber allows simultaneous detection of two different components (e.g. liquid mist and solid aerosol [1]), thus extending the potential of ICP-MS in radionuclide analysis. This presentation shows the application of the spray chamber for direct quantification of radionuclides on solid samples using laser ablation ICP-MS/MS. The difficult-to-measure radionuclide Sr-90 was directly quantified and visualized as a distribution image using online isotope dilution method.

[1] K Yanagisawa, M Matsueda, M Furukawa, H Ishiniwa, T Wada T Hirata, Y Takagai, Analyst 148 (2023) 4291-4299.

I029

GRAPHORMER-IR: GRAPH TRANSFORMERS CAN PREDICT EXPERIMENTAL IR AND IRMPD SPECTRA USING HIGHLY SPECIALIZED ATTENTION **Cailum M. K. Stienstra**[1], Liam Hebert[2], Teun van Wieringen[3], Patrick Thomas[1], Alexander Haack[1], Jason Guo[1], Jonathan Martens[3], W. Scott Hopkins[1,4,5] [1]Department of Chemistry, University of Waterloo, Waterloo, Ontario, N2L 3G1, Canada; [2]Cheriton School of Computer Science, University of Waterloo, Waterloo, Ontario, N2L 3G1; Canada [3]Radboud University, Institute for Molecules and Materials, FELIX Laboratory, 6525 ED, Nijmegen, The Netherlands; [4]Watermine Innovation, Waterloo, Ontario, N0B 2T0, Canada; [5]Centre for Eye and Vision Research, Hong Kong Science Park, New Territories, 999077, Hong Kong. (cmkstien@uwaterloo.ca)

Infrared (IR) spectroscopy is an important analytical tool in various chemical domains and a where in silico methods for predicting experimental spectra remain important. Here, we employ Graphormer, a graph neural network (GNN) transformer, to predict IR spectra using molecular structure using 53,528 high-quality spectra measured in five different experimental media. Using learned, augmented node embeddings generated from a novel feature encoder yields test scores to $SIS\mu$ = 0.8523 ± 0.0006, a total improvement of 19.7σ (t = 19) over the current state-of-the-art model Chemprop-IR ($SIS\mu$ =0.8409 ±0.0014, n = 5). These improved scores show how Graphormer-IR excels in capturing long-range interactions like hydrogen bonding, anharmonic peak positions in experimental spectra, and uncommon functional groups. Scaling our architecture to 210 attention heads demonstrates specialist-like behavior for distinct IR frequencies that improves performance. We further show that using transfer learning approaches and a small metabolite Infrared Multi-Photon Dissociation (IRMPD) spectral library from the FELIX Free Electron Laser (FEL) institute in the Netherlands, we perform the first ever accurate machine learning predictions of IRMPD spectra. This model will be used as a diagnostic pre-screening tool at WaterFEL, a future (open via application) user's facility at the University of Waterloo.

I030

HETEROGENEITY OF DELTA-8-TETRAHYDROCANNABINOL IN COMMERCIAL HEMP PRODUCTS. Christina Awwad and **Alison Holliday**, Moravian University, Department of Chemistry, 1200 Main Street, Bethlehem, PA 18017, USA. (hollidaya@moravian.edu)

While marijuana remains illegal on the federal level in the United States, hemp and hemp-derived products have been deregulated, provided that the concentration of delta-9-tetrahydrocannabinol (delta-9-THC) remains below 0.3%. As a result, there has been an explosion in the number of commercial hemp products containing psychoactive isomers of delta-9-THC, including delta-8-tetrahydrocannabinol (delta-8-THC). Using LC-MS, we have determined that there is large- and small-scale heterogeneity in the distribution of delta-8-THC in hemp product samples, as well as inconsistencies with reported commercial values.

I031

DETERMINATION OF RARE EARTH ELEMENTS (REES) AND PLATINUM GROUP METALS (PGM) IN FOODSTUFFS AT ULTRA-TRACE LEVELS BY ICP-MS/MS USING A HIGH EFFICIENCY SAMPLE INTRODUCTION SYSTEM.

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In the last decades, the use of rare earth elements and platinum group metals increased in different fields such us agriculture, medical technologies and in the manufacturing of hi-tech products. This may lead to an accumulation of these emergent contaminants in the food chain, which may have adverse effects on human health upon consumption of foodstuffs contaminated with these hazards. This work addresses the development of a multi-elemental method based on inductively coupled plasma-tandem mass spectrometry (ICP-MS/MS) using a high efficiency sample introduction system (APEXTM) for the determination of REEs and PGM at ultra-trace levels in food. For this purpose, the use of the mass shift detection mode (O2 reaction gas) was compared to the standard mode (no gas) to assess the optimum detection mode (high sensitivity and free of spectral interferences) for each analyte. In order to enhance the sensitivity for REEs and PGM ultra-trace determination, an APEXTM Ω was used. This sample introduction system provides significantly low limits of quantification compared to the conventional system. The method was validated and then applied to the determination of various REEs and PGM such us ruthenium, rhodium, palladium, osmium, platinum, thallium, lanthanum, cerium, gadolinium, neodymium etc. in a selection of foodstuffs.

I032 P

ASHES TO ASHES, DUST TO LUNGS: EXAMINING ELEMENTAL DISSOLUTION IN THE ATMOSPHERIC AGING OF DUST AND COAL FLY ASH USING ICP-MS.

Madison Smith[1], Arden Oglivie[1], Hind A. Al-Abadleh[2], and Nausheen Sadiq[1]. Mount Royal University, Department of Chemistry and Physics, 4825 Mount Royal Gate SW, Calgary, AB, T3E 6K6, Canada. [2]Wilfrid Laurier University, Department of Chemistry and Biochemistry, 75 University Ave W, Waterloo, ON, N2L 3C5, Canada. (msmit320@mtroyal.ca)

Many unanswered questions remain about the rate at which climate change is impacting our lives. It is important to understand atmospheric chemistry and its role in addressing climate change, air pollution, and environmental impact[1]. This study investigates atmospheric aging in dust and coal fly ash samples from the USA, India, and Europe, to understand the impact over time when exposed to acidic and organic conditions, which are chosen to promote surface-catalyzed reactions. Multi-elemental analysis of dust and coal fly ash samples will be conducted using an Agilent 7850 inductively coupled plasma-mass spectrometry (ICP-MS). This work focuses on arsenic (As), iron (Fe), copper (Cu), manganese (Mn), lead (Pb), zinc (Zn), and nickel (Ni) at pH 1 and 3 as these values show higher concentrations and cover a wider range of atmospheric particles/droplets. Previously, data has been collected for Day 14, focusing on only Fe. By expanding exposure time, data collection, and elements of interest, kinetic models for the rates of dissolution will be created from the initial exposure point, through 14 days. Improving kinetic modelling will allow for an accurate assessment of the atmospheric and environmental impacts of the trace elements.

[1] H. A. Al-Abadleh, Chem. Commun., 2024, 60, 1840-1855.

I033

CHEMICAL FUNCTIONALIZATION OF SYNTHETIC MELANIN FOR USE IN A FORENSIC SKIN SIMULANT. **Kgalalelo Rampete**[1], Jean-Paul Desaulniers[1,2], Theresa Stotesbury[1,2], [1]Applied Bioscience Graduate Program, Faculty of Science, Ontario Tech University, 2000 Simcoe St N, Oshawa, Ontario, L1G 0C5, Canada. [2]Faculty of Science, Ontario Tech University, 2000 Simcoe St N, Oshawa, Ontario, L1G 0C5, Canada. (kgalalelo.rampete@ontariotechu.net)

Skin simulants have been widely used in forensic research to investigate the properties of human skin at crime scenes. Previous research showed synthetic polymer materials were the most advantageous alternative as they can be tuned to mimic skin behavior. However, these materials lacked the optical and possible mechanical characteristics of skin imparted by melanin, a biomolecule, and pigment primarily responsible for UV absorbance and thermal regulation. We propose a new set of biomaterials, alginate-melanin polymers as candidate forensic skin simulants. Our current research explores the synthetic melanin functionalization and covalent immobilization to an alginate base material. Using propargyl bromide, we successfully reacted the amine moieties in melanin to yield melanin-modified propargyl groups and confirmed this using NMR spectroscopy, ATR-FTIR spectroscopy, and mass spectrometry. Broad-band absorption in the VIS region was observed using UV-VIS spectroscopy, confirming optical properties. We observed ATR-FTIR peak shifts at 2252 – 2292 cm^{-1}, together with a *m/z* of 394.3 from mass spectrometry indicating the alkyne's presence. Additionally, mechanical testing showed successful crosslinking of our polymers as they possessed the same optical properties. Consequently, this work supplements present synthetic biomaterials for forensic skin simulants and highlights the importance of incorporating biomolecules within such models.

I034 P

L-CYSTEINE-DRIVEN ANION-EXCHANGE HPLC SEPARATION OF Hg^{2+} AND $MeHg^{+}$: BIOINORGANIC AND ANALYTICAL PROSPECTS. **Negar Pourzadi** and Jürgen Gailer, Department of Chemistry, University of Calgary, AB, Canada. (pourzadi.negar@ucalgary.ca)

Due to the on-going contamination of the global environment with potentially toxic Hg species, there is an urgent need to obtain new insight into their metabolism in the bloodstream-organ system to better understand the bioinorganic basis of their chronic toxicological effects. To this end, we have - perhaps counterintuitively - employed anion-exchange (AEX) chromatography to investigate the pH-dependent retention behavior of Hg^{2+} and $MeHg^{+}$ using a 100 mM phosphate buffer with 10 mM L-cysteine (Cys) mobile phase in the pH range 5.0–8.0 using a Hg-specific detector. The results provide new insight into the coordination chemistry of these mercurials with Cys-ligands over this pH range. In addition, the results obtained at pH 7.4 represent a starting point to systematically investigate the effect of other small molecular weight dithiols and/or chloride (Cl^{-}) on the formation of novel Hg-containing metabolites. Last but not least, the results obtained at pH 5.0 serve as a basis for the development of a rapid baseline separation of these mercurials. Some preliminary results toward the development of an analytical method to separate these mercurials in <400 s will be presented.

I035

EVALUATION OF SHORT OLIGONUCLEOTIDE BOUND ALGINATE HYDROGELS USING CIRCULAR DICHROISM SPECTROSCOPY.

Daisee K. Lubrin[1], Jean-Paul Desaulniers[1,2], Theresa Stotesbury[1,2], [1]Applied Bioscience Graduate Program, Faculty of Science, Ontario Tech University, 2000 Simcoe St N, Oshawa, Ontario, L1G 0C5, Canada. [2]Faculty of Science, Ontario Tech University, 2000 Simcoe St N, Oshawa, Ontario, L1G 0C5, Canada. (daisee.lubrin@ontariotechu.net)

In this research, we developed an efficient and non-destructive method for analyzing an oligo-bound alginate hydrogel biosensor. Alginate is a biopolymer with efficacy as a low molecular weight hydrogel system. The functional groups present on the alginate molecule act as active sites and make it versatile and easily modified for subsequent reactions. A coupling reaction was used to bind an azide functionality to the alginate, then an alkyne-functionalized oligo was bound to the alginate-azide using a copper-catalyzed azide-alkyne cycloaddition click-chemistry reaction. FT-IR and NMR spectroscopy were used to characterize the biomaterials, and circular dichroism (CD) spectroscopy for functional analysis. For example, CD was used to assess full and/or partial binding of a suite of short oligos to the alginate hydrogel. PCA and LASSO were able to differentiate between single-stranded and double-stranded oligos, even in samples of mixtures containing a small number of non-complementary sequences. The oligo-bound alginate hydrogel has a limit of detection of 1.58 nmol and 0.76 nmol for DNA and RNA respectively. Overall, this alginate-based hydrogel provides a sensitive and specific method for the detection of oligos in aqueous solutions and demonstrates the potential for application to more complex sample matrices.

I036

EVALUATIONS OF TANDEM ELECTROSPRAY IONIZATION MASS SPECTROMETRY (ESI-MS/MS) OF NEURODEGENERATIVE-LINKED PEPTIDES.

Josephine Esposto[1], Robert J. Huber[2], Sanela Martic*[1,3] [1]Environmental and Life Sciences Program, Trent University, Peterborough, ON; [2]Department of Biology, Trent University, Peterborough, ON; [3]Department of Forensic Science, Environmental and Life Sciences Program, Material Science Program, Water Quality Center, Trent University, Peterborough, ON, K9L 0G2, Canada.

ESI-MS is a mass spectrometry ionization technique that enables transfer of intact molecular ions of biomolecules from solution into the gas phase [1]. Specifically, ESI can generate peptide ions and may preserve the peptide structure and their solution-based interactions into the gas phase [1,2]. Herein, we report on the analysis of peptides derived from the TDP-43 protein involved in neurodegenerative pathology (such as ALS disease). ESI-MS/MS analysis of wild-type, single Cys-to-Ala mutant, and double Cys-to-Ala mutant peptides was carried out. Various experimental parameters were tested, such as solvent composition, in order to optimize the ESI-MS method. The characteristic fragmentation patterns were also determined for all peptides. Data show that ESI-MS method is a viable tool for analysis of structurally similar peptides.

[1] D.D. Carlton Jr., K.A. Schug, Analytica Chimica Acta 686 (2011) 19-39.
[2] D.P. Donnelly, C.M. Rawlins, C.J. DeHart, L. Fornelli, L.F. Schachner, Z. Lin, J.L. Lippens, K.C. Aluri, R. Sarin, B. Chen, C. Lantz, W. Jung, K.R. Johnson, A. Koller, J.J. Wolff, I.D.G. Campuzano, J.R. Auclair, A.R. Ivanov, J.P. Whitelegge, L. Paša-Tolić, J. Chamot-Rooke, P.O. Danis, J.N. Agar. Nature Methods 16 (2019) 587-594.

I037 P

DETERMINATION OF CANNABIDIOL IN VARIOUS FLOWER BUDS USING LIQUID CHROMATOGRAPHY – MASS SPECTROMETRY. **Nicole Hanna**, Kingsley Donkor, Thompson Rivers University, Department of Physical Sciences (Chemistry), 805 TRU Way, Kamloops, B.C., V2C 0C8, Canada.

Due to recent legalization, consumption of cannabis products has increased, and can be dangerous for some if not labelled accurately. This research was conducted in order to determine the amount of cannabidiol (CBD) present in four cannabis flower bud samples with varying CBD concentrations: *Blue Iguana*, *Wappa*, *Mandarin Cookies* and *Miracle 15 x Alien Cookies*. Concentrations were determined using liquid chromatography - mass spectrometry (LC-MS). Prior to LC-MS analysis, CBD was extracted from the flower bud samples using methanol, and pre-concentrated by nitrogen evaporation. CBD was detected in higher quantities than labelled in 2 out of the 4 samples. The concentration of CBD present for *Blue Iguana* was 0.3450 ± 0.0618 mg/g; *Wappa* was 0.35501 ± 0.0445 mg/g; *Mandarin Cookies* was 0.0104 ± 0.0258 mg/g; *Miracle 15 x Alien Cookies* was 0.0941 ± 0.0243 mg/g. The precision of this study was acceptable with percent relative standard deviation ranging from 2.34% to 17.92%. The average percent recovery for cannabidiol was 80% for cannabis flower bud samples (n=4).

I038

BIOPHYSICAL ANALYSES OF DISEASE-RELATED PROTEINS: TDP-43, GELSOLIN AND CRYSTALLIN. **Josephine Esposto[1]**, Robert J. Huber[2], Sanela Martic[*1,3] [1]Environmental and Life Sciences Program, Trent University, Peterborough, ON; [2]Department of Biology, Trent University, Peterborough, ON; [3]Department of Forensic Science, Environmental and Life Sciences Program, Material Science Program, Water Quality Center, Trent University, Peterborough, ON K9L 0G2. (josephineesposto@trentu.ca)

The accumulation of misfolded proteins in the form of aggregates is linked to several diseases of the nervous system such as ALS, AD, PD, and prion diseases. The biophysical techniques, such as spectroscopy, microscopy etc. are ideally suited for study of aggregation and its inhibition [1]. Herein, we report on the analysis of proteins involved in ALS, amyloidosis, and cataract formation. Turbidity absorbance and Thioflavin T fluorescence spectroscopy, as well as transmission electron microscopy were used to characterize the protein structures [1,2]. The role of single-point amino acid mutations on the aggregation propensities was also evaluated. In addition, the inhibition of protein and peptides aggregates was achieved using small organic molecules and large antibodies. Overall, the data show that the aggregation process is unique to a protein which in turn can be targeted toward identification of viable therapeutics against neurodegenerative diseases.

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[2] Esposto JC, Martic S. Phosphorylated TAR DNA-binding protein-43: Aggregation and antibody-based inhibition. Biochim Biophys Acta Mol Basis Dis. 2021 Dec 1;1867(12):166234.

I039

DESIGN AND ELECTROCHEMICAL STUDIES OF NANOMATERIALS AND NANOCOMPOSITES FOR CLEAN ENERGY APPLICATIONS. **Aicheng Chen**, University of Guelph, Electrochemical Technology Centre, Department of Chemistry, 50 Stone Road East, Guelph, Ontario N1G 2W1, Canada. (aicheng@uoguelph.ca)

With rapidly mounting environmental concerns, coupled with the accelerated depletion of fossil fuels, there is a significant demand for the development of advanced technologies for sustainable energy production. Nanostructured materials with high surface areas have garnered significant interests due to their unique properties and impressive applications spanning electrocatalysis, photocatalysis, energy conversion and storage. Recently, our research team has designed and investigated a variety of functional nanomaterials. In this talk, the design and synthesis of advanced cobalt, palladium, ruthenium and graphene-based nanomaterials and nanocomposites are presented. The obtained nanomaterials and nanocomposites were studied by various surface characterization techniques (e.g., Raman spectroscopy, Fourier transform infrared spectroscopy, X-ray diffraction (XRD), high-energy XRD, scanning electron microscopy, transmission electron microscopy, energy-dispersive X-ray spectroscopy, and X-ray photoelectron spectroscopy) and electrochemical methods. The electrochemical properties of these nanomaterials as well as their promising applications in hydrogen production and storage are highlighted. The critical roles of nanostructured surfaces in the development of advanced electrochemical technologies for clean energy applications will be discussed.

I040

INTEGRATION OF A CAS12A-MEDIATED DNAZYME ACTUATOR WITH EFFICIENT RNA EXTRACTION FOR ULTRASENSITIVE COLORIMETRIC DETECTION OF VIRAL RNA. Huyan Xiao, JingYang Xu, Yanming Liu, Wei Feng, Bo Pang, Jeffery Tao, **Hongquan Zhang** Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, University of Alberta, Edmonton, Alberta T6G 2G3, Canada. (hongquan@ualberta.ca)

Developing highly sensitive and specific point-of-care (POC) tests is imperative to strengthen preparedness against future emerging infectious diseases. We present here the construction of a Cas12a-mediated DNAzyme actuator capable of converting the recognition of a specific nucleic acid sequence into an amplified colorimetric signal. To address viral RNA extraction challenges in POC and on-site applications, we developed a rapid and efficient method capable of lysing the viral particles, preserving the released viral RNA, and concentrating the viral RNA. The integration of the Cas12a-mediated DNAzyme actuator with the efficient RNA extraction and loop-mediated isothermal amplification enables a streamlined colorimetric assay for highly sensitive colorimetric detection of respiratory RNA viruses in gargle and saliva. This assay can detect as low as 83 viral particle/100 µL in gargle samples and 166 viral particles/100 µL in saliva samples. The entire assay was completed within 1 hour with a single controlled temperature. We demonstrated the application of the colorimetric assay to the detection of SARS-CoV-2 in 207 gargle and saliva samples collected from volunteers and achieved a clinical sensitivity of 95.1%. and specificity of 100%. The technique is adaptable for detecting specific nucleic acid sequences in other pathogens and suitable for resource-limited settings.

I041

AN NMR PERSPECTIVE ON THE MODULATION OF STRUCTURE AND DYNAMICS IN SOLIDS VIA DIRECTIONAL NON-COVALENT INTERACTIONS.

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In the first part of the talk, the role of multinuclear solid-state magnetic resonance in characterizing molecular, electronic, and crystal structures of halogen-bonded, chalcogen-bonded, tetrel-bonded, and pnictogen-bonded cocrystals will be discussed. Cocrystal engineering approaches developed in our laboratory are used to produce novel supramolecular architectures which are thoroughly analyzed via X-ray diffraction and solid-state NMR. These approaches include mechanochemical ball milling, resonant acoustic mixing, cosublimation, and more traditional solvent based techniques. Non-covalent bonds in these systems are probed via e.g., ^{13}C, ^{17}O, ^{19}F, $^{35/37}$Cl, ^{77}Se, $^{79/81}$Br, $^{121/123}$Sb, ^{125}Te, ^{127}I, and $^{185/187}$Re solid-state NMR and nuclear quadrupole resonance in the case of strongly quadrupolar isotopes. In the second part of the talk, we describe the results of a systematic study of the influence of halogen bonding to the nitrogen atoms of the model 2,3,5,6-tetramethylpyrazine molecule on the resulting cocrystalline architectures and rotational dynamics of its methyl groups. Using variable-temperature deuterium NMR relaxation measurements combined with single-crystal X-ray diffraction, we show how different halogen bond donors influence the crystal packing as well as the activation energy associated with methyl rotation. This work sheds light on the various subtle and competing steric and electronic effects which can influence molecular dynamics in these systems.

I042

TARGETED LC-MS/MS WORKFLOW FOR MEASURING QUANTITATIVE CHANGES IN THE TEAR PROTEOME.

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Proteins in tears play a central role in eye health and changes in some of these proteins has been shown to correlate with certain diseases. Quantitative analysis of tear proteins is a promising approach to identify biomarkers to help diagnose pathologies and help to better characterize the biological pathways involved. We have developed a non-invasive method to monitor changes in the tear proteome of healthy patients and those with eye diseases.

Using targeted LC-sMRM analysis, a method was developed for 226 consistently detected proteins. This list of proteins was first used to investigate inter-day and inter-individual variations in a healthy population. This work was useful in providing information to prioritize disease-related biomarkers, relative to their normal variations. This method was also used to investigate changes in tear proteome from patients with two ocular surface diseases: a rare multisystemic autoimmune disease, mucous membrane pemphigoid (MMP), and Sjogren's syndrome (SS), an autoimmune rheumatic disorder causing severe aqueous dry eyes. From both MMP and SS, several pathways were perturbed, including neutrophil degranulation and oxidative stress. Proteins secreted by the lacrimal gland were more enriched in SS, whereas extracellular matrix proteins were more implicated in MMP. Ongoing work includes further development of targeted assays of specific families of proteins in ocular fluids, including S100 and annexin proteins.

I043

PROTEOMICS APPROACHES IN DISCOVERY OF POTENTIAL ENZYMATIC BIOMARKERS FOR EARLY DIAGNOSIS OF BREAST CANCER. **Yingxi Li**[1, 2], Zoran Minic[1], Nico Hüttmann[1, 2], Suttinee Poolsup[1, 2], Rochelle D'Mello [1, 2], Maxim V. Berezovski[1, 2], [1] John L. Holmes Mass Spectrometry Facility, Faculty of Science, University of Ottawa, Ottawa, ON K1N 6N5, Canada; [2] Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, ON K1N 6N5, Canada.

Breast cancer (BC) is a leading cause of death in Canadian women. Early BC detection can greatly improve patient outcomes. However, a non-invasive BC detection method is not contemporarily available in clinics. Recent studies suggest that proteins in small extracellular vesicles (sEVs) could be promising biomarkers for non-invasive early-stage BC diagnosis. sEVs are membrane-enclosed vesicles secreted by cells, which drive different stages of carcinogenesis in BC. For proteomics analyses, sEVs were derived from different metastatic BC cell lines and a non-cancerous breast cell line. The results were generated from three proteomics approaches: quantitative proteomics, phosphoproteomics, and protein acetylation analysis. Enzymes with high abundances in cancerous cell lines were extracted from the quantitative proteomic data. Similarly, phosphorylated and acetylated enzymes present only in the cancer cell lines were extracted. Among these approaches, we proposed a list of enzymes, including their metabolic pathways, that can be potential BC biomarkers. Some of these phosphorylated and acetylated enzymes were validated, showing higher specific enzymatic activity in sEVs isolated from two metastatic BC cell lines (MCF7 and MDA-MB-231) when compared to a non-metastatic (MCF10A) cell line. Future validation of enzymes using both cancer cell lines and blood from BC patients remains to be determined.

I044

COMPLEMENTARITY OF LC- AND GC-ICP-MS FOR STUDYING TRACE ELEMENT CYCLING. Hakan Gürleyük and **Ben Wozniak**, Brooks Applied Labs, LLC, 13751 Lake City Way NE, Seattle, WA 98125, USA. (ben@brooksapplied.com, hakan@brooksapplied.com)

Understanding the environmental cycling of trace elements requires analytical methods capable of measuring their varied forms. While methods for the quantification of non-volatile species are generally available for many elements, those specifically targeting volatile forms remain less common. Since volatilization plays a key role in biogeochemical cycles and can be facilitated by anthropogenic activities (*e.g.*, landfill operations or wastewater treatment plants), methods targeting volatile species are important for better understanding how these processes may impact the environment and human health. Case studies will be presented showing how gas and liquid chromatography methods coupled to ICP-MS provide complimentary information for the study of volatile elements like arsenic, selenium, and sulfur. The additional insights provided by methods that can quantify multiple elements simultaneously will also be highlighted.

I045

EXPLORING QUADRUPOLE-CENTRAL-TRANSITION NMR SPECTROSCOPY FOR INVESTIGATING ALKALI METAL IONS IN SLOW-TUMBLING ENVIRONMENTS.

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Alkali metal ions play crucial roles in numerous biological and chemical processes, but their investigation using conventional Nuclear Magnetic Resonance (NMR) spectroscopy is impeded by the quadrupolar nature of their nuclei (e.g., ^{23}Na, ^{39}K, and ^{87}Rb all have I = 3/2 nuclei). Quadrupole-Central-Transition (QCT) NMR spectroscopy has emerged as a powerful tool for probing quadrupolar nuclei in solution, especially in slow-tumbling environments that mimic biological macromolecules [1,2]. This study explores the application of QCT NMR spectroscopy to investigate the behavior of alkali metal ions in slow-tumbling motion. By examining the QCT NMR signals of various alkali metal ions in these environments, we demonstrate that the restricted motion of the complexes leads to significantly narrower linewidths compared to those observed in aqueous solutions. This finding highlights the potential of QCT NMR spectroscopy for elucidating the behavior of alkali metal ions in biological macromolecules and unraveling complex chemical transformations. Our results provide insights into the behavior of alkali metal ions in slow-tumbling environments and their implications in biological and chemical systems, offering a basis for further investigations in related fields.

1. J. Zhu, G. Wu, J. Am. Chem. Soc. 133 (2011) 920-932.
2. G. Wu, Prog. Nucl. Magn. Reson. Spectrosc. 114/115 (2019) 135-191.

I046

ARSENIC SPECIATION IN WASTEWATER, PLANTS AND BIOFILMS AND EFFECTS ON REMOVAL IN LABORATORY-SCALE CONSTRUCTED WETLANDS.

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Twelve lab-scale wetlands divided into 4 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). More specifically, the goal of the study was to examine how arsenic speciation changed in the wastewater over time as well as examine the speciation of arsenic in the biofilms and plants to try and explain the differences in arsenic removal abilities for non-aerated and aerated systems. Our results showed that non-aerated mesocosms removed more arsenic than aerated mesocosms. Only non-aerated systems contained a higher proportion of methylated arsenic species likely due to microbial activity while speciation was unchanged for aerated systems by day 6 for weeks 1, 6 and 14. Only biofilms from non-aerated systems contained As(III)-S species and formed pyrite which both retained arsenic through precipitation and As(V) adsorption, respectively. Arsenic, sulfate and iron reducing bacteria in the non-aerated biofilms may have lead to the formation of As(III)-S precipitates and As(V) adsorbing pyrite. Although plants for non-aerated mesocosms removed more arsenic than aerated mesocosm, there was no clear pattern of arsenic speciation in the plants that would help explain arsenic removal.

I047

PROFILING POLYPHENOLS IN HONEYBEE PROPOLIS BY LC-MS.

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Propolis is a beehive product made of plant resins and bee's wax used to build the hive and protect it from invaders, including bacteria. Propolis is known to have anti-bacterial, anti-inflammatory and antioxidant properties due to its high polyphenol content and is thus used in natural medications, cosmetic products and as a food additive. The phenolic composition varies with geographical location, variability of resin sources available to the bees, and possibly by beekeepers' technique of collection. Samples of raw propolis and propolis processed into nutraceuticals (capsules, tinctures and sprays) from Canada and abroad were extracted in methanol with ultrasonication then analyzed for total polyphenol content based on the Folin-Ciocalteu spectrophotometric method. Phenolic profiles of extracts were acquired by LC-TOFMS (Agilent) or LC-Q-TOFMS (Waters) in negative ion mode, targeting a selection of polyphenolic species known to be abundant in brown, green, or red propolis. Semi-quantification was achieved using real or surrogate standards. Our goal was to identify correlations between LC-MS based phenolic profiles and total polyphenol content as a function of apiary location, year of propolis harvest, collection method, and processing. This presentation will describe the techniques used to characterize the propolis samples and present the observed correlations of polyphenol profiles and total content.

I048 P

MATERIAL CLASSIFICATION METHOD FOR STAINLESS STEEL SERIES USING MULTI-ELEMENT COMPONENT DATA OBTAINED BY ICP-MS IN PARTIALLY DISSOLVING MATERIALS.

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In quantitative analysis by ICP-MS, simultaneous multi-element analysis can be achieved quickly and easily. However, it is difficult to identify and classify materials from the quantitative values of inorganic ionic components in current analytical techniques. For example, stainless steel has a composition of mainly Fe, Cr and Ni; however, it is difficult to distinguish between this composition and a sample whose quantitative value agrees with it. In this study, a portion of a material such as stainless steel was dissolved and was applied to the multivariate analysis method to identify the classification of material. This approach was employed to classify the type of material that could not be determined by conventional analytical techniques. In this presentation, 42 materials were immersed in a pH10 solution (acetic acid-boric acid-phosphoric acid buffer solution; pH was adjusted with 2M NaOH), and the eluted components were quantitatively analyzed for 65 elements by ICP-MS. The quantitative values of 39 significant elements were used in hierarchical cluster analysis (HCA) and principal component analysis (PCA) to discriminate between basic austenitic stainless steel and stainless steel with special functions.

I049

ELUCIDATION OF DYNAMICS AND ENERGY LANDSCAPE OF MEMBRANE PROTEINS BY SOLID STATE NMR. Daryl Good, Peng Xiao, Philip Drewniak, Dylan Dingwell, Leonid Brown, Rachel Brown, Meaghan Ward, **Vlad Ladizhansky,** Department of Physics and Biophysics Interdepartmental Group, University of Guelph, 50 Stone Road E, Guelph, ON N1G2W1, Canada. (vladizha@uoguelph.ca)

Proteins are dynamic molecules which exist as conformational ensembles. Interconversion between conformational substates occurs either by means of thermal fluctuations or through functionally important motions. The substates were proposed to be organized as a hierarchical energy landscape, with individual energy valleys being separated by barriers whose heights depend on intra-protein interactions as well as on interactions with environment.

Here, we provide examples of how solid-state NMR could be used to probe the energy landscape of membrane proteins. In the first example, we use spin relaxation measurements to probe dynamics of a seven-helical membrane protein proteorhodopsin. We measured temperature dependence of relaxation rates and estimated activation energies of motional modes representing sidechain rotations, local backbone, and sidechain fluctuations as well as higher activation energy collective backbone motions.

In the second example, we use NMR-detected Hydrogen-Deuterium Exchange–to characterize the thermally induced unfolding of a membrane-embedded alpha-helical protein human aquaporin 1 (hAQP1). Its unfolding proceeds through an intermediate state to the misfolded state over two high activation barriers that define the overall protein stability. We show that in hAQP1, folding of loops kinetically stabilizes protein structure, in support of the notion of the third stage in the membrane protein folding model.

I050 P

RAMAN SPECTROMETRY OF DNA ISOLATED FROM FRUIT JAMS. **Carla Figueroa**, Kingsley Donkor, Thompson Rivers University, Department of Chemistry, Kamloops, BC V2E 2J1, Canada. (gaby.figue2001@gmail.com)

Rapid globalization of the international food market and the rise of genetically modified food make food quality control processes necessary to bring the best possible products to consumers. This can be done by studying DNA from foods like fruits and its derivatives. This project’s aim is to study DNA isolated from fruit jams using Raman spectrometry, a non-destructive analytical technique that provides information about chemical structure, impurity, and molecular interactions in a fast and less expensive way. It can identify a material or distinguish it from others based upon the interaction of light with the chemical bonds of the substance, revealing its “chemical fingerprint”. DNA information from fruits is important to learn more about how to improve crops so they are more resistant to disease, insect invasion, or climate change. As a result, fruit DNA can also be compared to other samples to determine if one of them has been altered in a way that might make a crop more nutritious or harmful. Normal and organic strawberry jams were obtained from a local grocery store, and their DNA was isolated using a DNA extraction kit. After the DNA extraction, samples were analyzed using Raman spectrometry to determine their “chemical fingerprint”.

I051 P

WAIT! IS THAT HUMAN SKIN? OPTIMIZATION OF ARTIFICIAL SKIN BY REFLECTING AGE AND ETHNICITY TO DETERMINE ELEMENTAL RISK ASSOCIATED WITH COSMETICS USING ICP-MS. **Lisa Tritz** and Nausheen Sadiq, Mount Royal University, Department of Chemistry, 4825 Mount Royal Gate SW, Calgary, ABT3E6K6, Canada. (ltrit251@mtroyal.ca)

Skin is the first defense against the outside world, continuously exposed to products such as creams, masks, and makeup, prompting the question: how can the safety of cosmetic products be assured? Cosmetic preparations have been shown to contain heavy metals such as lead, mercury, cadmium, arsenic and nickel[1]. Understanding the impacts of dermal heavy metal exposure is essential for developing robust regulations in the cosmetic industry. Previously, the permeability of heavy metals through skin was evaluated with a chitosan membrane that mimics human skin. This project aims to optimize the chitosan membrane to reflect a variety of ages and ethnicities, to comprehensively evaluate the permeability of these heavy metals, using ICP-MS. The suitability of the membranes for this experiment in representing “real skin” will be assessed by comparing them with Strat-M® membranes which have been shown to resemble human skin through permeability in vitro experiments [2].

[1] Borowska, S.; Brzóska, M. M. J. Appl. Toxicol. JAT 2015, 35 (6), 551–572.
[2] A. Haq; B. Goodyear; D. Ameen; V. Joshi; B. Michniak-Kohn, Int J Pharm., (2018) 547.

I052

DETECTION OF SMALL POLARONS IN ELECTROCHEMICAL MODULATED ELECTROCHROMIC TUNGSTEN OXIDE THIN FILMS. **B. Subramanian[a]**,M. MacCallum,[a] G. Gibson,[b] R. Irvine,[a] E. Steel,[a] [a] Department of Physics and Astronomy, Trent University, Peterborough, ON, Canada, 1600 W Bank Dr, K9L 0G2 [b] Nanofabrication Kingston, Department of Chemistry, Queens University, Kingston, ON, Canada, Innovation Park, 945 Princess St, K7L 0E9 (balajisubramanian@trentu.ca)

Electrochromic(EC) materials undergo reversible color changes (transparent ↔ blue) when small cations such as Li^+ are intercalated into their structure by the application of small potentials. In the colored state, they usually block IR radiation and transmit visible radiation, thus finding applications as energy savings materials. Herein, we report on the observed EC functionality in sputter deposited tungsten oxide (WO_3) thin films. To achieve this functionality, the WO_3 films were Lithated by electrochemical method. Optical properties in conjunction with Li ion intercalation/deintercalation of these films were studied by spectroscopic ellipsometry. The obtained optical constants could be fitted well with the small polaron absorption theory proposed by Bryskin [1] to decipher the mechanism of electrochromic coloration. Furthermore, a solid-state ion conducting layer was synthesized and EC-device prototypes were constructed. The detailed Li ion intercalation dynamics of the devices will also be discussed. The films were characterized by SEM and Raman spectroscopy for microstructure and crystalline structure respectively. We observed an optical modulation of about 68% for a wavelength of 750 nm which is suitable for applications in smart windows.

[1] V. V. Bryksin, Fiz. Tverd. Tela (Leningrad) 24, 1110 (1982); [Sov. Phys. Solid State 24, 627 (1982)].

I053

NEW INSIGHT FROM MEASUREMENTS OF THE BIO-ACCESSIBILITY OF ELEMENTS IN RICE USING THE CONTINUOUS ONLINE LEACHING METHOD WITH DETECTION BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY.

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

This presentation will review the continuous on-line leaching method (COLM) with real-time detection by inductively coupled plasma mass spectrometry (ICPMS) and its application to the risk assessment of As in rice before presenting new results that further our understanding of the risk associated with the consumption of rice by studying other elements than As. By utilizing the COLM and comparing results with a conventional sequential batch extraction method, a mixture of toxic (Cd and Pb) and essential elements (Cu, Fe and Zn) were studied in organic white, organic brown and basmati rice. The samples were maintained at 37 ºC during exposure to artificial saliva, gastric juice and intestinal juice. The released elements were determined by ICPMS. Both the COLM and the batch method showed over 60% bio-accessibility from the gastro-intestinal fluids in most instances. Cd and Pb levels were found to be higher than current interim reference levels provided by the Food and Drug Administration. The addition of a simple 5-min soak in water could reduce the concentration of toxic elements by up to 90%, indicating that all rice should be washed with clean water prior to consumption.

I054

VOLTAMMETRIC MEASUREMENTS IN A ROOM TEMPERATURE IONIC LIQUID USING SCANNING ELECTROCHEMICAL CELL MICROSCOPY.

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Scanning electrochemical cell microscopy (SECCM) uses a pipet probe to form a tiny meniscus droplet cell to carry out highly sensitive electrochemical measurements with high spatial resolution[1]. Room temperature ionic liquids (RTILs) have high viscosities and low vapour pressures compared to conventional solvents enabling the formation of a highly stable droplet at the end of a SECCM pipet probe [2]. The mass transport of a redox mediator in a RTIL is highly influenced by solvent viscosity which impacts its diffusion coefficient, and ultimately the voltametric response. While microelectrodes have been used to carry out voltametric measurements in RTILs and achieve a steady state response, this has not been explored in detail using SECCM. In this work, we will present our results that explore the effect of the pipet diameter, which influences the rate of mass transport, for a ferrocene redox mediator in the RTIL 1-butyl-3-methylimidazolium tetrafluoroborate to evaluate the conditions where a steady-state response can be achieved to enable the determination of the diffusion coefficient and heterogeneous rate constant at a glassy carbon substrate.

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

I055

SELECTIVITY OF ARSENOBETAINE USING FIELD PORTABLE X-RAY FLUORESCENCE.

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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.

I056

SOLID-STATE SPECIATION ANALYSIS USING SYNCHROTRON-BASED X-RAY ABSORPTION SPECTROSCOPIC METHODS.

Iris Koch, Blaire Coffey, David Patch, Antoine Hnain, Jennifer Scott, Ken Reimer, Kela Weber. Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 12 Verité Ave, 17000 Station Forces, Kingston, ON K7K 7B4, Canada. Andre Castillo. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. Debora Meira, Zou Finfrock. CLS@APS sector 20, Canadian Light Source Inc., 44 Innovation Boulevard, Saskatoon, Saskatchewan S7N 2V3, Canada. (koch-i@rmc.ca)

The necessity of determining the speciation of elements in understanding their toxicology, chemistry and environmental fate is undisputed. One of the difficulties in determining the speciation of elements in solid samples using conventional analytical methods is the complete characterization of the element, because extraction methods are usually required that may not be capable of removing all the element unchanged from the sample. Synchrotron-based x-ray absorption spectroscopy (XAS) can be used to examine samples in the solid state, both dried and fresh, often with cryogenic conditions to prevent chemical changes during analysis. We have used XAS in our group for many applications, including the speciation analysis of arsenic, silver, and other elements. The presentation will summarize recent developments in this area, including the feasibility of high energy resolution fluorescence detection for differentiation arsenic compounds

that normally have indistinguishable spectra when using x-ray absorption near edge structure analyses. An outreach study at the Advanced Photon Source investigating changes in the elemental speciation in socks will also be described.

I057

EMISSION FACTORS OF KEY AIR POLLUTANTS ARISING FROM BIOMASS BURNING.

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Biomass burning, including wildfires and wood combustion, generates large amounts of gaseous pollutants and particulate matter (PM) that significantly impact air quality, human health, and climatVaughe change. In this context, PM arising from Canadian wildfires contains substantial elemental carbon (EC) and organic carbon (OC). EC, a major component of soot, is a primary pollutant emitted during incomplete combustion, with strong light-absorbing properties that contribute to global warming. OC can be directly emitted or formed through atmospheric reactions and can scatter radiation, exerting a negative or positive climate-forcing effect.[1] Due to variations in emission factors based on fuel type and combustion conditions, there is limited data available on emissions from Canadian biomass sources. This study aims to quantify the emission factor of key air pollutants generated by burning pertinent fuels in the Canadian boreal forest, such as mulch and peat. Controlled biomass burning experiments were performed, including gas online measurements and the collection of quartz filters. These filters were subsequently analyzed using an OC-EC analyzer. The findings provide valuable data that can be input for accurate atmospheric models and predictions of wildfire environmental impacts.

[1] Li, W., & Bai, Z. Particuology (2009). (432–437)

I058 P

UNDERSTANDING THE CORRELATIONS BETWEEN HEAVY METALS AND MICROPLASTICS IN PLASTIC PACKAGED FOOD PRODUCTS. **Eliana Samara** and Nausheen Sadiq. Mount Royal University, Department of Chemistry and Physics, 4825 Mt Royal Gate SW, Calgary, AB, T3E 6k6, Canada. (esama092@mtroyal.ca)

North Americans have become highly dependent on processed and packaged food. The consumption of such foods may increase human exposure to microplastics (MP) [1]. Literature has shown that MPs adsorb toxins such as heavy metals, thereby increasing the health risk associated with MPs present in food [2]. This project examines heavy metals including aluminum, copper, and lead in plastic packaging used for fresh, raw, and canned food products. This research investigates correlations between various plastics, their color, and composition to better understand the relationship of microplastics at the elemental level. Samples were digested using microwave digestion and multi-elemental analysis was conducted using inductively coupled plasma- mass spectrometry (ICP-MS). The aim of the study is to have a deeper understanding of the risk associated with microplastics accumulation in the environment and in the human body. In addition, elemental fingerprinting will be investigated as a way to improve the identification of microplastics in the environment.

[1] S. Liu, J. Shi, J. Wang, Y. Dai, H. Li, J. Li, X. Liu, X. Chen, Z. Wang, & P. Zhang, Front. Microbiol., 12 (2021) 652520-652534.
[2] Q. Chen, H. Zhao, Y. Liu, L. Jin, & R. Peng, Toxics., 11(6) (2023) 490-510.

I059

ADDRESSING THE CHALLENGE OF SMALL MOLECULE SEPARATION IN COMPLEX SAMPLES THROUGH SUSTAINABLE AND HIGH-THROUGHPUT MICROEXTRACTION TECHNIQUES.

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The extraction of small molecules from complex samples presents a significant challenge in analytical method development, whether for targeted or non-targeted analysis. Recent trends in microextraction techniques development have shifted towards greener and faster approaches, ensuring sustainability and high throughput during the extraction process. Solid Phase Microextraction (SPME) is an ideal method that aligns with these features, offering simultaneous extraction and enrichment of targeted analytes. We explore novel microextraction methodologies to investigate the chemical composition of environmental and biological samples and assess the partitioning of small molecules in heterogeneous systems. Our work specifically targets various classes of environmental contaminants, such as PFAS, pesticides, and pharmaceuticals. We have developed specialized extraction technologies to ensure selective extraction and preconcentration of these compounds from complex samples before subjecting them to gas or liquid chromatography and direct introduction to mass spectrometry. These methods play a critical role in evaluating pollutants' environmental mobility and their impact on living systems. Additionally, we investigate the use of biocompatible extraction phases and alternative SPME geometries to address specific analytical needs while minimizing disturbances to partition equilibria during the extraction process. These advancements hold promise for improving the accuracy and efficiency of small molecule analysis in complex sample matrices.

I060

TRANSDERMAL WEARABLE SENSORS FOR MENTAL HEALTH ANALYTICS.

S. M. Mugo, W. Lu, S. Robertson, MacEwan University, Edmonton, Alberta, Canada. (*mugos@macewan.ca*)

In this presentation we will feature our flexible electrochemical probes based on biomimetric responsive composite hydrogels for in-situ multiplex detection of biologically relevant chemical markers, e.g., redox biomarkers, pH, biogenic amines, lactate, cortisol, and adrenaline. The composite hydrogels in these sensors simultaneously serve as an interface for biological fluid sampling and a medium for electrochemical sensing. In this presentation we will demonstrate results of our e-skin wearable sensors for real-time wireless monitoring of mental health biomarkers (emphasis on cortisol and adrenaline) in human sweat, towards applications in diagnostics in mental health and wellness. An accompanying emotional sensor app will be demonstrated.

[1] Mugo et al., *Talanta*, 2023, p.124531. doi.org/10.1016/j.talanta.2023.124531
[2] Mugo et al., *Biosensors*, *12*, 2022, p.854. doi.org/10.3390/bios12100854
[3] Mugo et al., *Microchimica Acta*, *189*, 2022, 206. doi.org/10.1007/s00604-022-05307-4

I061

DETECTING VOLATILE ORGANIC COMPOUNDS THAT MIMIC CADAVERIC DECOMPOSITION USING POLYDIACETYLENE-BASED COATINGS. **Deanna Fisher**, Simon Rondeau-Gagne, University of Windsor, Department of Chemistry and Biochemistry, 401 Sunset Ave, Windsor, ON N9B 3P4, Canada. (fishe11h@uwindsor.ca)

Polydiacetylenes (PDA) are a unique class of conjugated polymers that can be prepared from the topochemical polymerization of 1,3-butadiyne containing monomers. This polymer, composed of alternating ene-yne units, possesses rich optical properties that are used for sensing various analytes. PDA-based sensors mainly focus on colorimetric response or fluorescence of the polymer, where the materials can be classified as ‘active’ or ‘inactive’ phases, which can be utilized in a variety of applications. This immediate and sensitive optical change upon various stimuli or chemicals makes sensing with PDA a great option for in-field forensic utilization. Since forensic testing is often bulky, expensive, or requires training and expertise to use, a small and portable PDA-based sensor would revolutionize investigation. This presentation will focus on the utilization of PDA and optical sensing in the field of forensic science to examine volatile organic compounds (VOCs) released from cadaveric decomposition. With this new sensor platform that reacts to VOCs, we will discuss the sensing methodology and materials, along with post-mortem intervals, stage and rate of decomposition that can be determined by onsite forensics, before sending the body for further testing. Our new approach opens opportunities for the portable and accurate detection of VOCs in forensic science.

I062 P

IS THIS WHY I’M HAVING A BAD HAIR DAY? INVESTIGATING SCALP TRANSDERMAL DIFFUSION IN POPULAR HAIR PRODUCTS USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS). **Syrine Belaïd** and Nausheen Sadiq. Mount Royal University, Department of Chemistry and Physics, 4825 Mt Royal Gate SW, Calgary, AB T3E 6K6, Canada. (sbela250@mtroyal.ca)

The global hair care market is forecasted to hit $94 billion USD [1]. This highlights the widespread use of hair products, incorporated into daily, bi-weekly, or weekly routines. Despite their prevalent use, the regulatory framework surrounding the commercialization of these products is lacking in many countries. This study aims to address this regulatory gap by sourcing popular hair products dedicated to hair care and styling, such as shampoo, conditioner, hair gel, and mousse, for comprehensive elemental analysis. The primary focus will be on quantifying heavy metals present in these products using ICP-MS, providing foundational data to inform regulatory bodies in Canada, and around the world. Additionally, the extent to which these metals permeate through a chitosan-based membrane, designed to mimic human skin, will be measured. Elevated levels of heavy metals such as lead, mercury, and cadmium have been linked to adverse health effects ranging from skin irritation to neurological disorders. By elucidating whether these metals remain on the scalp or are rinsed away during normal use, we can better evaluate the safety and efficacy of these products for consumer use.

[1] M. Alda, Statista, (2024)

I063 P

CHITOSAN-BASED MEMBRANES FOR IN VITRO PERMEABILITY ANALYSIS OF TRACE ELEMENTS FROM COSMETIC AND PERSONAL CARE PRODUCTS USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS). **Birhan Gezahegn** and Nausheen Sadiq. Mount Royal University, Department of Chemistry and Physics, 4825 Mt Royal Gate SW, Calgary, AB T3E 6K6, Canada. (bgeza741@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 real-world factors such as multi-elemental exposure, chemical interactions, and varying exposure frequency. The development of in vitro study models for risk assessment of trace elements, especially their permeation across the skin 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. 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 membranes were designed to represent varying skin thicknesses which offers flexibility at low-cost while being biodegradable. Through modification and optimization of membrane thickness and composition, the aim of this model is to address the anatomical variations of skin relating to different body sites, age, sex, pigmentation, and health conditions.

I064

THE DETERMINATION OF NUTRITIONAL AND TOXIC ELEMENTS IN PLANT-BASED FOODS USING THE NEXION 2200 ICP-MS. **Sandeep Kumar,** Liyan Xing, Chady Stephan, and Aaron Hinemann, Perkin Elmer Scientific Canada ULC, 501 Rowntree Dairy Road, Unit # 6, Woodbridge, ON, L4L 8H1, Canada. (Sandeep.Kumar@PERKINELMER.COM)

Plant-based foods consumption and demand are on the rise due to their nutritional values and potential health benefits. These foods are made with ingredients derived from various sources such as fruits, nuts, vegetables, grains, and legumes. While plant-based foods offer many benefits, they carry some challenges associated with their formulation, nutritional content, and safety. Nutritional and toxic elements need to be routinely monitored in incoming raw materials and finished product, ensuring accurate label claims and compliance with quality control criteria per specified regulatory bodies. Inductively coupled plasma mass spectrometry (ICP-MS) is perfectly poised to achieve such a task, allowing the analysis of a wide range of elemental concentrations from ppm to ppt levels. In this work, PerkinElmer's NexION® 2200 ICP-MS was used to analyze a variety of plant-based food samples and several certified materials. A method for analyzing major and trace elements in plant-based food samples using the NexION 2200 ICP-MS equipped with a High Throughput System (HTS) is presented. The data quality was as evaluated per the QC criteria specified in the U.S. Food and Drug Administration (FDA) EAM 4.7 method.

I065 P

ANALYSIS OF TRACE ELEMENTS IN COASTAL SEAWATER USING THE NEXION 2200 ICP-MS.

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Seawater is one of the most challenging sample types to analyze by inductively coupled plasma mass spectrometry (ICP-MS) due to its high total dissolved solids (TDS) content in the matrix. Trace elemental analysis using ICP-MS has the advantages of multi-element analysis capability, high sensitivity, low detection limits, wide linear dynamic range, and easy automation. Nevertheless, ICP-MS analysis is also subject to interferences. The high concentrations of matrix components in seawater, such as sodium, magnesium, and chloride ions, may form polyatomic spectral interferences making the determination of trace elements, such as arsenic, cobalt, vanadium, and iron, challenging. Even for elements like cadmium, thallium, and lead, that have fewer spectral interferences, their low concentrations make them difficult to determine with accuracy and precision. Historically, for ICP-MS analysis of high TDS samples, several strategies have been employed, such as matrix separation, analyte preconcentration, reductive precipitation, hydride generation techniques, etc. These involve offline sample preparation and/or use of extra equipment. In this work, we present the direct analysis of seawater using a straightforward online dilution approach and using NexION 2200 ICP-MS equipped with High Throughput System (HTS). The data quality and instrument performance were evaluated by the method detection limits, the linearity, the accuracy, and long-term stability.

I066

AMBIENT MASS SPECTROMETRIC ANALYSIS OF ARCHIVED CLINICAL SAMPLES.

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Biobanks contain large collections of human tissue often as formalin-fixed paraffin-embedded (FFPE) and serve as an important resource for the study of disease and treatment. Analyzing FFPE tissues through mass spectrometry presents notable challenges, even though FFPE remains a preferred method for tissue preservation. To address these issues, a novel ambient ionization probe (i.e., HistoProbe) that incorporates a heated, modified version of the liquid microjunction-surface sampling probe (LMJ-SSP) was developed. The HistoProbe locally deparaffinizes the tissue sections during the analysis by solvating/melting and removing the paraffin at the probe/tissue contact point. Furthermore, the HistoProbe can operate in deparaffinization-only mode to replace the sample preparation technique and to prepare the FFPE tissue for further analysis. The probe is more environmentally sustainable using less than 1mL of ethyl acetate as the deparaffinization solvent compared to traditional approaches that required upwards of 50 mL of xylene. Additionally, when integrated into a 3D printer (Prusa i3 mk3), the HistoProbe doubles as an autosampler, guiding the probe with 50-micron (x, y, z) precision to target specific tissue regions of interest. This online/offline flexibility of the approach supports diverse ionization techniques for subsequent mass spectrometry analysis, such as desorption electrospray ionization and matrix-assisted laser desorption ionization.

I067

GOING AGAINST THE FLOW: COMPUTATIONAL AND EXPERIMENTAL INSIGHTS OF COUNTERFLOW SOLUTION FOR ADDRESSING CLOGGING CHALLENGES IN CONTINUOUS LIQUID MICROJUNCTION SURFACE SAMPLING PROBE. **Mina Alidoust**, Jian Yu, Richard D. Oleschuk. Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada. (21masl@queensu.ca, richard.oleschuk@chem.queensu.ca)

Liquid Microjunction Surface Sampling Probes (LMJ-SSP) combined with mass spectrometry offer a promising avenue for real-time and direct extraction of analytes from sample surfaces. One of the challenges faced in continuous sampling with LMJ-SSP is clogging. To address this, we propose a counterflow fluid approach, reversing the solvent delivery and analyte transport pathway using a dual-capillary system. To investigate the fluid dynamics behavior of the proposed flow regime at the probe-to-sample surface interface, a series of Computational Fluid Dynamics (CFD) simulations were conducted using COMSOL Multiphysics software. The simulations demonstrate that outlet capillary diameters, inlet flowrate, and outlet flow pressure fluctuations impact the fluid behaviour and clogging characteristics. Additionally, it was observed that the conventional probe configuration experiences a fluid flow decrease over time due to early particle accumulation, compared to the reverse probe. Experimental observations corroborate the modelling results indicating that while the conventional flow regime ceased functioning after a touches/extraction, the reverse flow method showed prolonged operation without clogging or carryover. This suggests that this approach can significantly extend the probe use for continuous monitoring/imaging. This study addresses LMJ-SSP clogging challenges and presents a practical solution through experimental validation and computational modeling optimization of the probe design.

I068

HAKUNA MATATA: HOW MICROPLASTICS, SUPERFUND SITES, AND COAL FLY ASH MAY MEAN SOME ELEMENTAL WORRIES. **Nausheen W. Sadiq**[1], Matthew Ross[2], Gwen O'Sullivan[3] and Hind A. Al-Abadleh[4]. [1]Mount Royal University, Department of Chemistry and Physics, 4825 Mount Royal Gate SW, Calgary, AB, T3E 6K6, Canada. [2]5-138P, City Centre Campus, 10700-104 Avenue, Edmonton, AB, T5J 4S2, Canada. [3]Mount Royal University, Department of Earth and Environmental Science, 4825 Mount Royal Gate SW, Calgary, T3E 6K6, Canada. [4]Wilfrid Laurier University, Department of Chemistry and Biochemistry, 75 University Ave W, Waterloo, ON, N2L 3C5, Canada. (nsadiq@mtroyal.ca)

The circle of life when it comes to elements, compounds, and chemicals seems to last till death do us part. With many chemicals being made to last longer than humans, it is important to understand their elemental impact in a variety of contexts. This study analyzes various microplastics, samples from superfund sites, as well as dust and coal fly ash samples at the elemental level using an Agilent 7850 inductively coupled plasma - mass spectrometry (ICP-MS). This will allow for further understanding of their impact on human health and the environment. Focus is placed on a variety of both toxic and essential elements including: aluminum (Al), arsenic (As), cadmium (Cd), copper (Cu), iron (Fe), nickel (Ni), vanadium (V), lead (Pb), and zinc (Zn). By understanding the impact elements in these matrices can have on the environment, a more robust understanding of elements' points of entry in the food chain, interactions in the human body, and exposure mitigation strategies can be developed.

I069

MICROPLASTICS ANALYSIS AND CHARACTERIZATION IN ENVIRONMENTAL SAMPLES. **Sandy Zhao**, Shimadzu (Mandel), 2 Admiral Place, Guelph, ON N1G 4N4, Canada.

Microplastics, tiny plastic particles measuring just a few micrometers, pose significant risks to marine ecosystems and human health. Despite increasing research, the full extent of their environmental impact remains unclear, emphasizing the need for innovative analytical methods. Advancement in physical characterization techniques such as IR/Raman microscopy and quantitative pyrolysis-GCMS is presented. These methods offer complementary insights in the hope to contribute to the development of effective strategies for mitigating the impact of microplastics pollution.

I070

COPPER ISOTOPIC COMPOSITION OF ISOLATED CERULOPLASMIN FROM HUMAN SERUM **Kerri A. Miller[1]**, Arnie Charbonneau[1] Patrick L. Day[2], Anthony Maus[2], Paul J. Jannetto[2], Sunil Q. Mehta[3], Mukesh K. Pandey[2], Michael E. Wieser[1], [1]Cancer Institute, University of Calgary, 2500 University Drive NW, T2N 1N4, Calgary, AB, Canada; [2]Department of Laboratory Medicine and Pathology, Mayo Clinic, Rochester, MN, United States, 55905; [3]PrairieCare Medical Group, Rochester, MN, United States, 55905.

Copper stable isotope composition of blood serum has provided valuable insights into alteration of copper processing due to a disorder or disease. One persistent challenge is understanding the mechanism for these changes, which in living systems is the result of changes in binding sites available for the metal. Here we have developed an immuno-purification procedure for ceruloplasmin using antibody-coated magnetic beads to measure the isotopic composition of ceruloplasmin in human blood serum. We have assessed the isotopic composition of this protein and compared to the bulk serum and residual serum after ceruloplasmin removal. We tested this procedure in male and female adults, and in children between the ages of 2-4 years old with autism spectrum disorder and healthy age-matched controls. In adults, the measured isotopic composition of ceruloplasmin is consistent with theoretical predictions for those specific binding sites. In the children the measured isotopic composition did not match the theoretical predictions and indicate other factors driving the isotopic fractionation observed for ceruloplasmin in this age group. The ability to characterize the isotopic composition of individual proteins will be a critical tool to understand metal-protein interactions.

I071 P

NORMALIZATION OF VIRAL LEVELS IN WASTEWATER THROUGH THE USE OF HUMAN BIOMARKERS. **Jordan Rensing**[1], Stephen Brown[1], Simon van der Plas[1], Sarah Jane Payne[2], Hridaynath Bhattacharjee[2], Julie Jia[2], [1]Queen's University, Department of Chemistry, 90

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Wastewater based epidemiology is used to monitor disease levels in the community, particularly SARS-CoV-2, without subjecting people to mass testing. However, normalization is required to ensure more accurate data, correcting for variation in fecal content in sewage due to dilution. Identifying the best biomarker to use for normalization is therefore important to get the best results. For this purpose, this study looks at a few biological and chemical biomarkers and evaluates their use as normalization markers in comparison to the existing pepper mild mottle virus (PMMoV) biomarker, currently used in many wastewater monitoring programs. Initially, E coli was tested compared to PMMoV, with poor performance. Currently, we are testing chemical markers, including caffeine and cholesterol, to determine if they are more effective than PMMoV.

I072

GOLD ANALYSIS BY PORTABLE LASER-INDUCED BREAKDOWN SPECTROSCOPY AND THE CHALLENGE OF THE NUGGET EFFECT.

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Laser-induced breakdown spectroscopy (LIBS) presents significant potential for the gold mining industry, offering cost-effective, rapid, on-site quantitative elemental analysis of ores. However, challenges are posed by the nugget effect, a natural phenomenon common in gold deposits characterized by high variability of gold grade distribution. This variability arises from the intricate mineralization characteristics of gold-bearing systems, including small-scale grade variation, low-continuity structures, varying grain sizes, and particle clustering. To mitigate the magnitude of the nugget effect, it is imperative to implement sampling protocols informed by thorough mineralization knowledge and rigorous analytical procedures. This study investigates the influence of the nugget effect on LIBS analyses employing a portable prototype, the ProspectOre™, developed for assaying low gold concentrations. By scrutinizing factors such as the beam spot size, number of laser shots, particle size, and gold heterogeneous distribution, the study aims to elucidate the role of sampling protocols in minimizing the nugget effect. Furthermore, a calibration curve derived from certified reference materials was produced to accurately quantify ore samples from the Canadian Malartic and Barnat open pit mine and the underground Odyssey mine. This research will present sampling strategies to recognize and reduce the nugget effect when measuring gold, underscoring the potential of LIBS in supporting gold mining operations.

I073

INVESTIGATING AN ANALYTICAL METHOD FOR QUANTIFYING TETRAHYDROZOLINE FOUND IN EYE DROPS USING CAPILLARY ELECTROPHORESIS. **Malika Sharma**, Thompson Rivers University. Kingsley Donkor, Thompson Rivers University, Department of Chemistry, 805 TRU Way, Kamloops, BC V2C 0C8, Canada. (malikasharma741@gmail.com)

The objective of this study is to develop and optimize an analytical method using capillary electrophoresis (CE) to isolate and determine tetrahydrozoline in commercially available eye drops. Eye drops are saline solutions with medications in them to treat various eye diseases. They are used as artificial tears to treat dry eyes or simple irritation such as itching or redness. One of the main components of eye drops is tetrahydrozoline, a decongestant used to relieve redness in the eyes caused by minor eye irritations (ex: smog, swimming, dust, smoke). Unfortunately, recently the oral consumption of eye drops has risen causing poisoning due to the tetrahydrozoline in the eye drops. Factors such as concentration, pH, and type of background electrolyte will be investigated to determine the optimum conditions for the CE analysis. Furthermore, the CE method will be validated to evaluate its precision, accuracy, and limits of detection and quantification. The findings of this study will provide insight into the successful detection of tetrahydrozoline from commercially available eye drops to identify which brands of eye drops are potentially unsafe. It will also provide the eye drop industry with a better means to ensure that their products contain the correct amount of tetrahydrozoline.

I074

TOWARDS A NO-WASH ELECTROCHEMICAL IMMUNOASSAY FOR 25-OH VITAMIN D_3. **Aaliya Pathan**, Darius Rackus, Department of Chemistry and Biology, Toronto Metropolitan University, 350 Victoria St., Toronto, ON M5B 2K3, Canada,; Institute for Biomedical Engineering, Science, and Technology (iBEST), St. Michael’s Hospital, Toronto, ON M5B 1W8, Canada; Keenan Research Centre for Biomedical Science at St. Michael’s Hospital, Toronto, ON M5B 1W8, Canada; Graduate Program in Molecular Science, Toronto Metropolitan University, 350 Victoria St., Toronto, ON M5B 2K3, Canada.

Vitamin D3 deficiency is highly prevalent, making it one of the biomarkers for several chronic diseases. As a result, there has been a demand for portable testing platforms to enhance disease management and monitoring accessibility. Currently, determination of vitamin D levels relies on laboratory-based immunoassays which face challenges such as interference through non-specific adsorption and the need for washing to remove unbound labels, making it complex and time-consuming. To address this challenge, we report a wash-less electrochemical competitive immunoassay to measure free 25-OH Vitamin D3 (25-OHD). The assay is based on passivation of the electrode surface resulting in a decrease in electron transfer for the reduction of $Ru^{3+/2+}$. Cyclic voltammetry and electron impedance spectroscopy were used to interrogate the electrode surface in response to varying concentrations of 25-OHD. In a one-pot “no-wash” protocol, a limit of detection of 30 ng/mL was observed. The no-wash assay was improved by orienting capture antibodies immobilized on the electrode surface through protein A or by replacing the capture antibody with VDBA14 aptamer. While further reduction of signal-to-noise is needed for a lower LOD, these findings demonstrate the potential for a rapid, simple electrochemical, and quantitative point-of-care test for vitamin D.

I075 P

GIVE ME A BREAK - TRACE ELEMENTAL ANALYSIS OF KITKAT CHOCOLATE BARS AND WRAPPERS USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS).

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Who doesn't love a sweet treat? KitKat, valued at approximately 2.12 billion US dollars [1], produces a variety of candy bars, wrapped in foil packaging. Metals can leach out from materials, such as packaging by diffusion into the solids or liquids they are in contact with. This raises concerns on the composition of food packing materials, such as candy bar wrappers. Multiple scenarios were tested with KitKats, including different wrappers, increased storage temperature, as well as expired bars left in their wrappers for extended periods of time. Trace multi-elemental analysis was conducted using ICP-MS; and up to 3 ppm of aluminum was observed in the chocolate. Aluminum accumulation can lead to harmful impacts on bone metabolism and brain functions [2]. The risk is higher in younger populations, thus posing an even greater concern to children, who are the main consumers of chocolate products. Understanding the leaching of potentially toxic elements from food wrappers into consumable products will help in creating better safety standards in the packaging industry. X-ray photoelectron spectroscopy (XPS) will be explored to further examine the elemental content in wrappers.

[1] Kit Kat brand value 2022. Statista.
[2] Sedman, A. Pediatr. Nephrol. 6(4) (1992) 383-393

I076

DROPLETS OF JUSTICE – TRACE METAL ANALYSIS OF SWEAT AND SALIVA SAMPLES TO DETERMINE SEX, ETHNICITY, AND AGE IN FORENSIC SCIENCE USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY (ICP-MS).

Aimee Williams, Madison Smith and Nausheen Sadiq. Mount Royal University, Department of Chemistry and Physics, 4825 Mount Royal Gate, Calgary, AB T3E 6K6, Canada. (awill623@mtroyal.ca).

Is all evidence created equal? For decades, analytical tools have been used to analyze forensic evidence [1]. Past studies have used hair to determine sex and ethnicity while utilizing the power of ICP in forensic research [1]. This study aims to investigate the use of trace metal analysis of sweat and saliva samples as a viable and reliable forensic identification tool. This study uses ICP-MS to analyze elements present in sweat and saliva samples, and uses multivariate statistics for the determination of sex, ethnicity, and age. Preliminary testing (n=30) has shown success rates of 70-96% in determining age, ethnicity, and sex. Age is a variable that has not yet been tested in this context. This study focuses on improving past results by increasing sample size, optimizing sample collection, and assessing sample stability. This will be done by collecting from a larger pool of participants and working to enhance signals across elements of interest. Finally, the stability of samples will be tested on various surfaces to determine the extent of degradation, over a period of time, equivalent to what may be seen at a crime scene.

[1] Huang, L.; Beauchemin, D. J. Anal. At. Spectrom. 29 (2014) 1228-1232.

I077

INTERFACIAL INSIGHTS: PROBING POLYMER CONFORMATIONS WITH SFG SPECTROSCOPY.

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Polymer thin films are widely used in biomedical applications, microelectronics, specialized coatings, and membranes. The interfacial region between the film and its surroundings significantly impacts macroscopic properties, including crystallization, adhesion and wettability. The ability to probe, control and tailor the conformation of these interfacial chains becomes crucial for ensuring the applicability and stability of thin films across various applications. Through innovative applications of SFG spectroscopy, our research established correlations between chain molecular weight, thermal and mechanical sample history, interfacial chain conformation, and macroscopic polymer properties. Our three key research avenues are: 1. Investigating the influence of polymer molecular weight (Mw) on molecular conformation near highly interactive substrates [1]; 2. Analyzing the differences in polymer conformations across various interfaces (e.g. polymer/air and polymer/substrate) and their influence on the polymer dewetting behavior [2]; and 3. Broadening the scope of SFG spectroscopy applications to address new analytical challenges, such as determining the surface lamellar orientation of semi-crystalline polymers [3]. These insights offer a foundation for future studies in polymer science and materials engineering, driving advancements in thin film technology and applications.

[1] de Lima, B.M.; Hayes, P.L.; Wood-Adams, P.M., *Langmuir* 37 (2021), 10036.
[2] de Lima, B.M.; Hayes, P.L.; Wood-Adams, (2024) in preparation.
[3] de Lima, B. M.; Hayes, P. L; Wood-Adams P. M., *Anal. Chim. Acta* 1248 (2023), 340904.

I078

LATEST ADVANCES IN NEOMA MC-ICP-MS/MS ISOTOPIC ANALYSIS,

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Copper and zinc are important metals that exhibit distinct isotopic fractionations as a result of various physical, chemical and biological processes. As a result, copper and zinc isotopes have been widely used in a range of applications, varying from cosmochemistry to medical metallomics. In this application note, we discuss the various application spaces for copper and zinc isotopes and show the capabilities of the Neoma MS/MS MC-ICP-MS for measuring these isotope systems at high precision.

I079

THE MOLECULAR RELATIONSHIP BETWEEN SOIL POREWATER CARBON, VEGETATION COVERAGE, AND GREENHOUSE GAS PRODUCTION IN THAWING NORTHERN PEATLANDS.

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Northern peatlands are changing rapidly due to rising temperatures and releasing greenhouse gases like methane (CH_4). Since decomposing vegetation is the main source of dissolved organic matter

(DOM) in soil porewaters, the type of vegetation and molecular characteristics of organic carbon may affect microbial metabolism and CH_4 release as these ecosystems thaw, but little work has explored these ecological and molecular patterns. We used a combination of spectroscopy and Fourier Transform ion Cyclotron Resonance Mass Spectrometry (FT-ICR-MS) to evaluate the optical and molecular relationships between porewater DOM across bogs, fens, and peatland plateaus in the Northwest Territories, Canada. We found that peatlands contained significantly greater proportions of highly unsaturated compounds than other regions, whereas bogs contained more unsaturated aliphatic compounds. Peatlands with greater *Sphagnum* moss and graminoid coverage enhanced the production of unsaturated aliphatic molecules. As the proportion of unsaturated aliphatic molecules in soil porewater DOM increased, so did CH_4 concentrations, likely due to the production of microbially accessible DOM. Conversely, ecosystems with high shrub and gross primary productivity led to lower CH_4 concentrations, likely due to more aromatic and biologically inaccessible DOM. These findings show the importance of vegetation, DOM and carbon cycling in northern ecosystems under global change.

I080

EXPLORING THE MICROSCOPIC LANDSCAPE OF MOFS: INSIGHTS INTO METAL CENTERS, ORGANIC LINKERS, AND GUEST MOLECULES FROM SOLID-STATE NMR.

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Metal-organic frameworks (MOFs) are a new generation of porous materials known for their unique properties like modularity, tunable pore sizes/functionality, high surface area, and permanent porosity. Despite their diverse applications, certain key aspects such as local structures, specific molecular-level features, and guest behavior are not well understood. Solid-state NMR is a powerful tool for characterization, providing nuclide-specific information complementary to X-ray diffraction. This technique helps researchers gain insights into MOF structures at a molecular level, including guest molecule behavior, essential for optimizing their applications. In this talk, I will provide an overview of our work on MOF characterization via both high-resolution and wide-line solid-state NMR. The focuses will be on (1) probing metal center environments by interrogating ^{67}Zn, ^{91}Zr, $^{65/63}$Cu, ^{209}Bi, via their NMR spectra. The NMR results permit us to refine the local bonding geometry of a metal center, examine the disordering around metal ions, and resolving multiple inequivalent metal sites; (2) examining local structure around organic linkers by ^{17}O high-resolution NMR, and chlorine/iodine in halide-organic hybrid MOFs by ^{35}Cl and ^{127}I wide-line NMR; (3) monitoring the behavior of guest molecules. The NMR results lead to a deeper understanding of the structure-properties-function relationships in MOF systems.

I081

MAXIMIZING ICP-OES WORKFLOW EFFICIENCY WITH THE ALL-NEW AGILENT ADVANCED DILUTION SYSTEM (ADS2).

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The effectiveness of an inductively coupled plasma optical emission spectrometry (ICP-OES) analytical run relies heavily on the meticulous manual tasks executed by the analyst. Among these critical tasks are the preparation of calibration standards and sample dilution prior to the run. These processes can be labor-intensive and time-consuming, and carry the risk of introducing contaminants and errors, potentially compromising the quality of the results. Additionally, samples that are identified to be overrange in concentration during the analysis would require further dilution, which can be disruptive to the analyst's daily workflow. To help labs reduce sample turnaround time and minimize cost per analysis, Agilent introduces the Advanced Dilution System (ADS 2). This is an online dilution system, purpose-built for Agilent ICP-OES (and ICP-MS) instruments. The ADS2 can automatically prepare multipoint calibration standards from a single stock standard, dilute samples before analysis by a prescribed factor, and dilute and remeasure sample immediately when sample concentration overrange is detected. Online autodilution and automatic calibration standards preparation not only reduce manual labor but also avoid the risk of introducing human error and contamination during sample preparation. The ADS2 provides valuable support for less experienced operators in conducting routine analyses, streamlines the ICP-OES workflow and ensures accurate analytical results.

I082

ADVANCING LASER-INDUCED BREAKDOWN SPECTROSCOPY FOR SOIL MONITORING.

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Laser-induced breakdown spectroscopy (LIBS) is a high-speed, waste-free technique based on the application of an intense laser pulse to produce a plasma on a material surface and the measurement of resultant emitted light to determine elemental composition. The adoption of LIBS devices for agricultural applications requires addressing challenges associated with signal variability, matrix effects, and reliable characterization of low concentration nutrients and contaminants. Here, we present our work applying LIBS to assess carbon content in soils, obtaining a limit of detection of 0.34-0.5 w/w% using the second harmonic of an Nd:YAG nanosecond pulsed laser [1]. We further investigate the impact of soil preparation on spectroscopic analysis, performing a comprehensive qualitative and quantitative study on soils prepared as ground moist, air-dried with clumps, and ground air-dried, finding that moist and ground soils could be accurately classified using machine learning techniques. Finally, we present an adaptive learning machine learning technique to improve LIBS classification accuracy using limited experimental data. These advancements support the development and application of a portable LIBS device for in-situ soil analysis.

[1] S. Mohajan et al., Optics Express 31, 20 (2023)
[2] Y. Huang et al., IEEE Transactions on Plasma Science 51, 9 (2023)

I083 P

MULTI-ELEMENT ANALYSIS OF DRINKING WATER FOLLOWING ISO 17294-2 USING THE NEXION 1000 ICP-MS.

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Elemental analysis is critical to ensuring the quality and safety of drinking water. The international standard method ISO 17294 outlines the analysis of elements in water samples such as drinking water, surface water, groundwater, wastewater, and eluates using inductively coupled plasma mass spectrometry (ICP-MS).

The NexION® 1100 ICP-MS is equipped with Universal Cell Technology (UCT) that can be operated in both Collision mode with kinetic energy discrimination (KED) and Reaction mode with dynamic reaction cell (DRC) to tackle the polyatomic interferences. Compared to its prior generation, the NexION 1100 ICP-MS allows a higher cell gas flow, which can be utilized to mitigate the argon dimer interference on the measurement of Se in Reaction (DRC) mode using a premixed helium-hydrogen gas mixture.

The NexION 1100 ICP-MS is also advanced with integration of the LumiCoil™ RF coil technology with a GreenCT ™ cooling system that reduces cooling needs, an LCD touch screen for a PC-less experience as well as LED lighting to alert users of the instrument's running status, and the all new Syngistix™ software for ICP-MS.

I084

PROSTATE CANCER RESHAPES THE SECRETED AND EXTRACELLULAR VESICLE URINARY PROTEOMES. Amanda Khoo[1,2], Meinusha Govindarajan[1,2], Zhuyu Qiu[3], Lydia Y. Liu[1,2], Vladimir Ignatchenko[2], Matthew Waas[2], Andrew Macklin[2], Alexander Keszei[2], Brian P. Main[4], Lifang Yang[4], Raymond S. Lance[5], Michelle R. Downes[6], O. John Semmes[4], Danny Vesprini[7], Stanley K. Liu[1,7], Julius O. Nyalwidhe[4], Paul C. Boutros[1,3], **Thomas Kislinger**[1,2]
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Urine is a complex biofluid that reflects both overall physiologic state and the state of the genitourinary tissues through which it passes. It contains both secreted proteins and proteins encapsulated in tissue-derived extracellular vesicles (EVs). To understand the population variability and clinical utility of urine, we quantified the secreted and EV proteomes from 190 men, including a subset with prostate cancer. We demonstrate that a simple protocol enriches prostatic proteins in urine. Secreted and EV proteins arise from different subcellular compartments. Urinary EVs are faithful surrogates of tissue proteomes, but secreted proteins in urine or cell line EVs are not. The urinary proteome is longitudinally stable over several years. It can accurately and non-invasively distinguish malignant from benign prostatic lesions, and can risk-stratify prostate tumors. This resource quantifies the complexity of the urinary proteome, and reveals the synergistic value of secreted and EV proteomes for translational and biomarker studies.

I085

PROBING HYDROGEN BONDING INTERACTIONS BY SOLID-STATE ^{17}O NMR. **Gang Wu**. Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (wugang@queensu.ca)

Hydrogen bonding is one of the most important driving forces in many chemical and biological processes [1]. While spectroscopic and structural characteristics of hydrogen bond formation in molecular systems have been well documented in the literature, new information continues to emerge whenever a new analytical probe is employed. Because oxygen is ubiquitous in hydrogen bonds, ^{17}O (I = 5/2, natural abundance 0.037%) NMR was to be a particularly sensitive probe for studying hydrogen bonding interactions even in the early days of NMR [2-4]. However, progress has been rather slow over the past several decades due to technical difficulties in detecting ^{17}O NMR signals. In recent years, we have used solid-state ^{17}O NMR to probe hydrogen bonding interactions in many cases [5,6]. In this talk, we will show several examples where solid-state ^{17}O NMR is used to provide several important aspects of hydrogen bonding interactions.

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[2] J. Reuben, A. Tzalmona, and D. Samuel, *Proc. Chem. Soc*. (1962) 353.
[3] A. E. Florin and M. Alei, *J. Chem. Phys*. 47 (1967) 4268.
[4] J. Reuben, *J. Am. Chem. Soc*. 91 (1969) 5725.
[5] G. Wu, *Prog. Nucl. Magn. Reson. Spectrosc*. 114/115 (2019) 135.
[6] J. Palmer and G. Wu, *Annu. Rep. NMR Spectrosc*. 103 (2021) 1.

I086

ANALYSIS OF FORTIFIED FOODS USING ICP-MS. **Jenny Nelson**, Agilent Technologies (jenny.nelson@agilent.com)

This presentation is about the analysis of fortified foods such as infant formula and meal replacement drinks, which are worth billions of dollars every year. The regulations for such foods vary by country, and they specify minimum and maximum levels of essential minerals and potentially harmful trace elements. We will share our simple and robust quantitative analysis of 28 elements using single quadrupole ICP-MS.

Regulators have established high standards for safety and nutritional value, especially for infants, as excessive or insufficient iodine consumption can lead to thyroid problems. Iodide (I-) is more bio-available than iodate (IO3-), which affects the nutritional status of iodine in food. Elemental speciation separates iodide and iodate from iodine (I2) and organic forms of iodine to determine a food's toxicity and health benefits. We will also share the Simultaneous Iodine and Bromine Speciation Analysis of Infant Formula by HPLC-ICP-MS determination of four halogen species in less than 6.5 minutes.

I087

DO SURFACTANTS REALLY ASSIST TRYPSIN DIGESTION? AN ASSESSMENT OF CUMULATIVE ENZYME ACTIVITY SAYS OTHERWISE. **Alan Doucette**[1], & Jessica Nickerson[2], [1]Department of Chemistry, Dalhousie University, Halifax, Nova Scotia; [2]Allumiqs Corporation, Halifax, Nova Scotia, Canada.

Multiple reports have demonstrated that certain solution additives, such as surfactants, will enhance enzymatic activity when added at specific concentrations [1]. However, our group has recently shown that enhanced enzyme activity may be short lived, as kinetic assays demonstrate an accelerated decline in sustained trypsin activity [2]. Here, we discuss the impacts of surfactants (sodium dodecyl sulfate, SDS; sodium deoxycholate, SDC), previously employed in surfactant-assisted proteomics workflows to enhance proteome analysis. Although low surfactant concentrations (0.01% SDS or 0.2% SDC), significantly enhances the initial trypsin activity, time course spectroscopic enzyme activity assays revealed accelerated enzyme deactivation, with a 10 to 40-fold reductions in enzyme activity half-life. Quantitative mass spectrometry analysis of a proteome extract, digested with surfactants, consistently revealed a decreased peptide count and lower signal intensity, indicative of lower digestion efficiency compared to a non-surfactant control. Furthermore, detergents did not improve detection of membrane proteins, nor hydrophobic peptides. These results stress the importance of assessing cumulative enzyme activity when optimizing the digestion of a proteome mixture, particularly in the presence of denaturants.

[1] T. Masuda, M. Tomita, Y. Ishihama. *J. Proteome Res.* 7 (2008) 731–740.
[2] J. Nickerson, A. Doucette. *Biology.* 11 (2022) 1444.

I088

QUANTITATIVE ASSESSMENT OF EQUILIBRIUM-CONSTANT ACCURACY. Tong Ye Wang,[1] Jessica Latimer,[1] Isaac Kogan,[1] Svetlana M. Krylova,[1] Sebastian Schreiber,[2] Philip Kohlman,[2] Joachim Jose,[2] and **Sergey N. Krylov**[1], [1]Department of Chemistry, York University, Toronto, Canada M3J 1P3; [2]Institute of Pharmaceutical and Medicinal Chemistry, University of Münster, Münster, Germany 48149

Nonlinear regression, utilized to compute equilibrium constants, can produce precise but grossly inaccurate values due to unknown systematic errors in variables [1-4]. Here, we present the first approach to quantitatively assess the accuracy of such equilibrium constants. This approach combines regression stability analysis with error propagation analysis. To help the scientific community quickly adopt this approach, we have developed an accuracy calculator and implemented it as a user-friendly web app: aci.sci.yorku.ca. As assessing the accuracy of equilibrium constants is now possible and simple, we recommend that this assessment be adopted as a standard for publishing equilibrium constants characterizing biomolecular binding, enzymatic reactions, adsorption, etc.

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I089

AI INTEGRATION IN FTIR SPECTROSCOPY: ENHANCING QUANTIFICATION, **Daniel Vetter**, Anton Paar GmbH

How can Artificial Intelligence (AI) advance the capabilities of Fourier Transform Infrared (FTIR) spectroscopy? FTIR spectroscopy is known for identifying substances and measuring analytes.

We'll look closely at how AI methods can improve the accuracy of quantification in spectral analysis. We examine Partial Least Squares (PLS) models, a standard tool in FTIR analysis, highlighting both their strengths and limitations. Additionally, we compare PLS models with neural networks, assessing their respective advantages and disadvantages.

The comparison shall provide insights into the effectiveness of each approach. Furthermore, diverse applications of neural networks in FTIR spectroscopy are discussed, extending beyond quantification.

The presentation shall provide a clear examination of how AI methods can refine quantification in FTIR spectroscopy, offering practical insights into the integration of PLS models and neural networks within this scientific field.

I090

DEVELOPMENT OF A NEW METHOD TO DETERMINE MACRO- AND MICRONUTRIENTS IN BARLEY FORAGE SAMPLES USING LASER-INDUCED BREAKDOWN SPECTROSCOPY (LIBS). **Andressa Adame**[1,2], Francis Vanier[2], Allan Fuertado[3], Mohamad Sabsabi[2], François Vidal[1], [1]Institut National de la Recherche Scientifique, Centre Energie Matériaux Télécommunications, 1650 Lionel-Boulet blvd., Varennes, QC J3X 1S2, Canada ; [2]National Research Council of Canada, Clean Energy Innovation Research Center 75 de Mortagne Blvd., Boucherville, QC J4B 6Y4, Canada; [3]National Research Council of Canada, Aquatic & Crops Resource Development, 110 Gymnasium Place, Saskatoon, SK S7N 0W9, Canada. (andressa.adame@inrs.ca)

Laser-Induced Breakdown Spectroscopy (LIBS) has been established as a reliable and efficient alternative to conventional analytical methods. It is a versatile analytical technique that enables multi-elemental analysis of solid samples in a faster way, and it has been considered an excellent tool for assessing nutritional content of plant material. In this presentation, we will present the development of the method to analyze the elemental composition of barley forage using LIBS. First, different instrumental configurations and experimental parameters were evaluated in order to optimize the determination of macro- (Ca, Mg, K, P, N) and micronutrients (Fe, Zn, Mn) in the samples. Then, 61 barley forage samples were analyzed using the developed method. This presentation will focus on the method optimization studies and the results obtained for barley forage samples.

[1] Arantes de Carvalho GG, *et al*. Recent advances in LIBS and XRF for the analysis of plants. *J. Anal. At. Spectrom*. 33 (2018) 919–944.

I091

HIGH PRECISION STRUCTURES OF CELLULOSE POLYMORPHS OBTAINED WITH AN NMR CRYSTALLOGRAPHIC APPROACH. **Darren Brouwer**, Department of Chemistry, Redeemer University, Ancaster ON, Canada. (dbrouwer@redeemer.ca)

Detailed structural characterization of cellulose has presented numerous challenges due to its fibrous nature and multiplicity of crystalline forms. Although determining its structure(s) has been the focus of much effort, there remain outstanding questions, particularly concerning the hydrogen-bonding networks within and between cellulose chains. Fibre neutron and X-ray diffraction (XRD) experiments have provided structures for the various forms of cellulose, however there are intrinsic limitations to the precision that can be achieved with fibre diffraction. ^{13}C solid-state NMR (SSNMR) has played a vital role in detecting the existence of polymorphism in cellulose, but the structural information accessible by ^{13}C SSNMR has not been fully exploited. Here, it is shown that an “NMR crystallography” approach, in which SSNMR results and DFT calculations are combined, provides high precision structures of four of the polymorphs of cellulose.

I092

AN OVERVIEW OF THE LIBS DEVELOPMENT AND THE FUTURE OF IMPROVING ITS SENSITIVITY BY COMBINATION WITH OTHER TECHNIQUES. **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], A. Adame[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)

As LIBS enabling tools (such as pulsed lasers, detectors and spectrometers) have rapidly evolved in the recent years, LIBS has seen significant advances and expanded adoption in geology, planetary science, defence, food, environment, industry, mining, biology, etc. Meanwhile, extensive research has been carried out to improve LIBS sensitivity and performance through the use of several approaches such as the double pulse mode, resonant LIBS, nanoparticles enhanced LIBS (NELIBS), combining LIBS with Laser-Induced Fluorescence (LIF) or infrared (IR), microwave, spark, Raman or XRF among other techniques. The analytical performance of LIBS for a multi-elemental analysis now achieves a level that is equal to, or even in some cases better than, that of classical methods. Improving the LIBS sensitivity involves several strategies aimed at enhancing the signal-to-noise ratio and increasing the detectability of analytes. In this presentation, we will highlight the new emerging approaches aiming at improving the LIBS sensitivity and its analytical figure of merit with the most significant research contributions for quantitative analysis by LIBS carried out in our laboratory and elsewhere. Finally, a personal viewpoint on the LIBS development and the future of its combination with others techniques will be given.

I093

LASER-INDUCED BREAKDOWN SPECTROSCOPY AND INFRARED SPECTROSCOPY FOR THE RAPID AND ACCURATE ANALYSIS OF THE COMPOSITION OF PLANTS.

Jinan Sabsabi[1], Andressa Adame[1], Mohamad Sabsabi[2] , Francois Vidal[1], Francis Vanier [2] , Aissa Harhira[2] [1]Institut National de la Recherche Scientifique, Energy, Materials and Telecommunications Centre, 1650 Lionel-Boulet Blvd, Varennes, QC, Canada ; [2]National Research Council of Canada, 75 Mortagne Blvd, Boucherville, QC, Canada.

In agriculture, rapid and accurate nutrient analysis is critical to optimizing yields. Direct spectroscopy techniques not requiring sample preparation such as laser-induced breakdown spectroscopy (LIBS) or infrared spectroscopy (IR), with their its simplicity and effectiveness, offers an advantageous alternative to traditional methods that are labor-intensive, costly and require skilled personnel. In this work, we use IR and LIBS techniques to measure protein content and elemental composition of barley samples. Our long-term goal is to develop a user-friendly analyzer that can be used in the field by non-experts to measure relevant parameters in real time. Both methods can be performed with compact instruments and require only simple sample preparation. Initially, we focused on barley samples previously analyzed by conventional methods to calibrate our instruments. The complexity of the spectra obtained requires the use of multivariate mathematical methods (chemometrics) that allow the calibration of spectral measurements from extensive data across the spectra. The methods we have used include partial least squares (PLS) and artificial neural networks. This talk will focus on our experimental results, the implementation of the chosen chemometric methods, in particular the data preprocessing steps, and the promising results obtained and their comparison to those of traditional methods.

I094

DEVELOPMENT OF LC-FAIMS-MS/MS FOR THE CHARACTERIZATION OF ACINETOBACTER BAUMANNII.

Jacek 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)

Mass spectrometry (MS) is a powerful technology to characterize bacterial lipids. Our recent development in coupling MS to high-field asymmetric waveform ion mobility spectrometry (FAIMS) allowed us to study the alteration of mouse serum lipidome after Acinetobacter baumannii inoculation. In this presentation, we further optimized the FAIMS parameters, including compensation voltages and chromatography gradients, for analysing different subclasses of lipids, such as phosphatidylcholine (PC), phosphatidylethanolamine (PE), phosphatidylserine (PS), phosphatidylinositol (PI), and phosphatidylglycerol (PG), bis(monoacylglycero)phosphate (BMP), N-acyl-phosphatidylethanolamine (NAPE), lyso-N-acyl-PE (LNAPE), cardiolipin (CL) and lipid A. With the separation offered by HILIC, we were able to characterize isomeric structures between PG and BMP, PE and LNAPE. Moreover, we characterized the lipid A structures from different strains and a new subclass of phospholipids, i.e., phosphatidyl-acyl-glycerophosphoethanolamine (PAGPE). We have demonstrated that the proposed NPLC-FAIMS-MS/MS is a dependable technique for characterizing bacterial lipidomics.

I095

ANALYSIS OF PALLADIUM IN ROCK ORE BY LASER-INDUCED BREAKDOWN SPECTROSCOPY (LIBS) AND CHARACTERIZATION OF THE MORPHOLOGY OF LASER-PRODUCED CRATERS.

S. Selmani[1], I. Elhamdaoui[1], M. Sabsabi[2], M. Constantin[3], P. Bouchard[2], F. Vidal[1], [1]Institut national de la recherche scientifique, Centre Énergie Matériaux Télécommunications, 1650 Lionel-Boulet Blvd., Varennes, QC J3X 1P7, Canada; [2]National Research Council Canada, 75 de Mortagne Blvd., Boucherville, QC J4B 6Y4 Canada; [3]Université Laval, Département de géologie et de génie géologique, 1065 Ave de la Médecine, Québec, QC G1V 0A6, Canada.

Geologists are interested in rapidly characterizing and measuring the concentration of platinum group elements in rocks at mine sites. LIBS is an emerging technique in geochemistry that allows rapid in situ analysis of elemental and mineralogical composition. This work demonstrates the analytical applicability of LIBS as an analyzer for assessing the palladium content in different types of ores. Three types of palladium-bearing ores with different mineralogy were analyzed by LIBS: two with high Ni-Cu-(PGE) and Fe contents (36% and 22.5% iron) and the third type from the Si-rich deposit with low iron content (~5% iron) from the Lac des Îles palladium mine (Ontario, Canada). To calibrate the LIBS instrument, we used three sets of certified reference materials in the form of compressed powders with a quasi-homogeneous palladium concentration ranging from about one part per million (ppm) to 500 ppm. The palladium concentration was determined by LIBS using the Pd line at 348.115 nm and the average Pd concentration was compared with that obtained by conventional chemical analysis. In addition, optical coherence tomography (OCT) and scanning electron microscopy (SEM) were used to study the crater morphology in the three major phases of a palladium ore fragment (plagioclase feldspar, amphibole, and sulfides).

I096

AN NMR-GUIDED METHOD FOR REFINING AND CORRECTING CRYSTAL STRUCTURES.

James K. Harper, Ryan Toomey, Brigham Young University, Department of Chemistry and Biochemistry, Provo, UT, 84602, USA. (jim.harper@byu.edu)

An NMR-guided process for refining crystal structures is described. This approach employs a lattice-including DFT relaxation followed by Monte Carlo sampling to create new atom positions. Candidates having the best agreement between experimental and computed ^{13}C or ^{15}N NMR shift tensors are selected for further refinement and this process is repeated until convergence. Several non-NMR metrics, examined before and after refinement, indicate that this process does not introduce structural errors. Unfortunately, planewave DFT computations are costly, and an alternative has recently been developed involving clusters of molecules. This new approach requires that strong interaction (e.g. hydrogen bonding) be explicitly included and represents more distant fields with the polarized continuum model. This methodology provides more accurate computed NMR parameters than planewave methods (e.g. GIAPW) and is achieved at a lower computational cost. At present, our refinement techniques have only been used on benchmark structures and the feasibility of making genuine structural correction has not been demonstrated. Very recently, work has been completed to demonstrate that these refinement tools are also superb at identifying structural errors and correcting them. Two examples of such improvements will be presented and result in a reassignment of space group and a significant rearrangement of hydrogen bonding.

I097

FULL AND SURFACE PROTEOMICS OF EXTRACELLULAR VESICLES. Nico Hüttmann, Yingxi Li, Suttinee Poolsup, Emil Zaripov, Rochelle D'Mello, Vanessa Susevski, Zoran Minic and **Maxim V. Berezovski**, Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, ON K1N 6N5, Canada. (maxim.berezovski@uottawa.ca)

We identified exosomal proteins GLUT-1, GPC-1, and ADAM10 as potential biomarkers for breast cancer. Additionally, enzymes such as OAT, TALDO1, and BLMH in microvesicles were linked to cancer therapeutics. Further phosphoproteomic and acetylation analyses of the full proteome of cancer-derived exosomes revealed enzymes indicative of cancer progression. In addition to full proteomics, we analyzed the surface proteome of breast cancer EVs and found 11 potential protein biomarkers that may be involved in early breast cancer diagnosis.

I098

IDENTIFICATION, QUANTIFICATION, AND CHARACTERIZATION OF HUMAN POLYCLONAL ANTIBODIES. Zoe Turner, Yasmine Rais, Weize Tang, Zhiqiang Fu, and **Andrei P. Drabovich**, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, University of Alberta, Edmonton, AB T6G 2R3, Canada. (drabovic@ualberta.ca)

Recent advances in proteomics facilitated the development of selective, sensitive, and reproducible assays for quantification of low-abundance proteins in biological samples [1-2]. Here, we will present the development of immunoaffinity–mass spectrometry (IA-MS) assays for quantification of the endogenous polyclonal antibodies in blood serum and characterization of antibody isotypes (IgG, IgA, IgM, IgE, IgD) and subclasses (IgG1-4, IgA1-2). IA-MS assays revealed relatively high levels (>1 µg/mL IgG1) and pathogen-specific diversity of serum polyclonal antibodies against SARS-CoV-2 [3] and Respiratory Syncytial Virus [4] antigens. Autoantibodies against prostate-specific antigens were detected at substantially lower levels (<10 ng/mL). Profiling of the repertoire diversity of variable chains revealed the use of several dozen IGHV genes in polyclonal antibody response. The presented IA-MS assays will facilitate the comprehensive characterization of the endogenous polyclonal antibodies, rational design of serological testing, and precision approaches in immunology.

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[2] Fu Z et al. *Mol. Cell. Proteomics* 2021, 20, 100075
[3] Fu Z et al. *Anal. Chem.* 2022, 94, 12990–12999
[4] Weize T et al. *bioRxiv* 2023, 10.1101/2023.10.27.564451.

I099

DETECTING PROTEIN INTERACTIONS BY CO-FRACTIONATION-MASS SPECTROMETRY: PUSHING SENSITIVITY AND CROSS INTO NON-MODEL SPECIES.

Leonard Foster, University of British Columbia, 2125 East Mall, Vancouver, BC V6T 1Z4, Canada. (foster@msl.ubc.ca)

Proteins generally function through interactions with other proteins, so understanding how a cellular system works depends on being able to detect these interactions accurately and efficiently. Co-fractionation-mass spectrometry (CF-MS) is a method for detecting proteome-wide protein–protein interactions that relies on proteins in a complex moving together through a separation gradient, using mass spectrometry to measure the chromatograms or electropherograms of all proteins. While sensitive, accurate, and higher-throughput than traditional affinity capture methods for detecting protein interactions, CF-MS works best when there are some known interactions that should be detected that can be used to calibrate the analysis. I will discuss recent lessons learned from a meta-analysis of all previous CF-MS experiments and then our efforts to use machine learning to bring this approach to non-model systems where fewer or no true interactions might be known.

I100

CAPILLARY ELECTROPHORESIS-MASS SPECTROMETRY FOR TOP-DOWN PROTEOMICS.

Liangliang Sun, Department of Chemistry, Michigan State University, 578 S Shaw Lane, East Lansing, MI 48824, USA. (lsun@chemistry.msu.edu)

Capillary electrophoresis-mass spectrometry (CE-MS) has been recognized as a promising analytical tool for top-down characterization of proteoforms since 1980s. We recently showed several cases of applying advanced CE-MS techniques to the delineation of proteoforms. First, we performed the first TDP study of a pair of isogenic human nonmetastatic and metastatic colorectal cancer (CRC) cell lines (SW480 and SW620) using CE-MS/MS.[1] We identified 23,622 proteoforms of over 2000 genes from the two cell lines, representing nearly fivefold improvement in the number of proteoform identifications compared to previous TDP datasets of human cancer cells. We revealed substantial transformation of CRC cells in proteoforms after metastasis. Second, we developed a CE-ion mobility spectrometry (IMS)-MS/MS technique for online multi-dimensional separation of proteoforms for the first time and showed that the technique could substantially improve the identification of large proteoforms (>30 kDa) in complex samples.[2] Third, we applied CE-MS-based TDP to characterize nanoparticle protein corona in a proteoform-specific manner for the first time to advance nanomedicine.[3] Lastly, we developed native CE-MS technique to probe the endogenous protein complexes in complex biological samples with the detection of up to 400 kDa protein complexes from an *E. coli* cell lysate.[4]

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I101

SEPARATION OF FLUORESCENT ORGANIC DYES AND SALTS BY CAPILLARY ELECTROPHORESIS TO INVESTIGATE THEIR BINDING PROPERTIES WITH METAL OXIDE NANOPARTICLES, NANOPLASTICS, CASEIN MICELLES, AND LIPOSOMES.

Edward P.C. Lai, Amos Onomhante. Carleton University, Department of Chemistry, 1125 Colonel By Dr, Ottawa, ON K1S 5B6, Canada. (edward.lai@carleton.ca)

The motivation for this work was to utilize capillary electrophoresis for the separation of organic dyes and salts in our investigation of their binding properties with various metal oxide nanoparticles, nanoplastics, casein micelles, or liposomes present in water samples. The free dyes/salts were separated from each other and the dye/salt-bound nanoparticles, thus eliminating any potential interference and guaranteeing high accuracy in the % binding determination. Our strategy was to use laser-induced fluorescence (LIF) for the detection of all dyes/salts, thus enabling high-throughput analysis for screening environmental water samples. Experimental results have been obtained in our lab that verify binding of rhodamine 6G dye and acridine orange salt with transition metal oxide nanoparticles, polystyrene nanospheres, casein micelles, and soy lecithin liposomes. Two diode lasers were operated at l_{ex} of 450 and 480 nm, together with interference filters collecting emission photons with l_{em} from 520 to 580 nm, to facilitate the simultaneous detection of several dyes/salts. The dual LIF detectors could be placed at two detection windows along the fused silica capillary, thus permitting flexible adjustment of the migration times for overlapped dye/salt peaks in the electropherogram. This analytical approach could potentially be expanded to employ multiple LIF detectors with fiber optics.

I102

INVESTIGATING THE BINDING PROPERTIES OF METAL OXIDE NANOPARTICLES, NANOPLASTICS, CASEIN MICELLES, AND LIPOSOMES WITH FLUORESCENT ORGANIC DYE AND SALT.

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The motivation for this work was to develop a laser-induced fluorescence technique for the direct analysis of various metal oxide nanoparticles, nanoplastics, casein micelles, or liposomes present in water samples. Our strategy involved the addition of a fluorescent dye/salt to each sample for binding with the target analytes. The % binding, based on a decrease of the dye/salt fluorescence intensity due to quenching, depends on the number of surface binding sites on each analyte. This new approach enables high-throughput analysis for screening environmental water samples, based on the fast binding kinetics and rapid measurement of fluorescence emission intensity. Experimental results have been obtained in our lab to verify binding of rhodamine 6G dye and acridine orange salt with transition metal oxide nanoparticles, polystyrene nanospheres, casein micelles, and soy lecithin liposomes. Binding percentages as high as 98(±2)% were attained for the liposomes when using a dye/salt concentration of 125 mg/mL, a diode laser operated at l_{ex} of 480 nm, and an interference filter collecting only emission photons with l_{em} of 580 nm. Capillary electrophoresis was employed to separate the free dye/salt from the dye/salt-bound liposomes, thus eliminating any potential interference and guaranteeing high accuracy of % binding determination within 10 min.

I103

MONITORING PROTEIN-PROTEIN INTERACTIONS IN LIVING, DYING, AND INFECTED CELLS. **Olivier Julien**, University of Alberta, Department of Biochemistry, 4-020C Katz Group, Edmonton, AB T6G 2H7, Canada.

Proteases regulate key biological processes, such as apoptosis, cell differentiation and viral infections. The dysregulation of caspases, for example, underlies several human diseases including cancer and autoimmunity. A better understanding of these enzymes is therefore of great interest toward the design of new therapies and improved elucidation of disease mechanisms. One key step towards our understanding of protease functions is through the identification of their substrates. In short, we use a rationally engineered peptide ligase enzyme called *subtiligase* to attach biotinylated ester peptide probes to free *N*-termini, allowing site-specific identification and quantification of cleavage sites in complex mixtures by LC-MS/MS. Using functional proteomics approaches, we aim to identify protease substrates and find ways to modulate their proteolysis and associated biological processes. Proteomics results identifying hundreds of apoptotic and non-apoptotic caspase substrates will be presented, as well as proteolysis occurring in virus infected cells.

I104

QUANTITATIVE ANALYSIS OF CHLORINE IN CEMENT STANDARD SAMPLES WITH LASER INDUCED BREAKDOWN SPECTROSCOPY**. I. Elhamdaoui[1],** S. Selmani[1], M. Sabsabi[2], M. Constantin[3], P. Bouchard[2], F. Vidal[1], [1]Institut National de la Recherche Scientifique, Centre Énergie Matériaux Télécommunications, 1650 Lionel-Boulet Blvd., Varennes, QC J3X 1P7, Canada; [2]National Research Council Canada, 75 de Mortagne Blvd., Boucherville, QC J4B 6Y4 Canada; [3]Université Laval, Département de géologie et de génie géologique, 1065 Ave de la Médecine, Québec, QC G1V 0A6, Canada.

Laser-induced breakdown spectroscopy (LIBS) has shown great promise for the quantitative analysis of chlorine in cement samples, offering rapid measurement with minimal sample preparation [1]. This presentation details the results obtained in our laboratory aimed at assessing the reliability and accuracy of Cl measurements by LIBS under a variety of experimental and methodological conditions. The results showed that LIBS could effectively quantify Cl in cement with an average relative error generally below 10%. However, performance varied considerably depending on the adopted normalization approach, due to differences in measurement protocols and data analysis methods. In this presentation, we will explain the complete LIBS analysis protocol that contributed to the good obtained accuracy of our results and good prediction of unknown standard samples comparison with results obtained by conventional techniques with results

[1] Tobias Völker, Gerd Wilsch, Igor B. Gornushkin, Lucie Kratochvilová, Pavel Pořízka, Jozef Kaiser, Steven Millar, Gábor Galbács, Dávid J. Palásti, Patrick M. Janovszky, Shuzo Eto, Christoph Langer, Gesa Kapteina, Marcus Illguth, Jenny Götz, Marina Licht, Michael Raupach, Ismail Elhamdaoui, Mohamad Sabsabi, Paul Bouchard, Lev Nagli, Michael Gaft, Yosef Raichlin, Luis Javier Fernández-Menéndez, Cristina Méndez-López, Nerea Bordel, Cassian Gottlieb, Christian Bohling, Riccardo Finotello, Daniel L'Hermite, Céline Quéré, Matthias B. Lierenfeld, Spectrochimica Acta Part B 202 (2023) 106632.

I105

10-SECOND LIPIDOMIC ANALYSIS WITH PICOSECOND INFRARED LASER MASS SPECTROMETRY TO DIAGNOSE BRAIN CANCER TYPES. Alexa Fiorante [1], Michael Woolman[1], David Munoz[2], Gelareh Zadeh[3,4], Sunit Das[2,4], Contributors to the Unity Health Brain Biobank[2], Taira Kiyota[5], Ahmed Aman[5], Howard Ginsberg[2,4] and **Arash Zarrine-Afsar[1,3,4]** , [1]Department of medical biophysics, University of Toronto; [2]Unity Health Toronto; [3]Princess Margaret Cancer Centre; [4]Department of Surgery, University of Toronto; [5] Ontario Institute for Cancer Research, Canada.

Surveys of neurosurgical outcome data have suggested suitable extents (aggressiveness) of resection to improve survival for many brain cancer types. Personalization of the extent of resection relies on highly subjective intraoperative diagnoses wherein the depth of the diagnostic information depends on the level of experience of the pathologist. Picosecond InfraRed Laser Mass Spectrometry (PIRL-MS) uses picosecond bursts of mid-infrared laser radiation to extract, in a non-thermal manner, tissue lipids (1) present in cellular membranes, giving cells and nuclei their unique shapes (utilized in morphometric pathology with staining & microscopy) and (2) altered in tumorigenesis due to cross-talk with cellular signalling in metabolism (potentially also revealing cancer molecular subtypes in 10 seconds as shown) for real-time profiling of molecular content unique to each tumour type. Close to 1,300 frozen brain cancer specimens over 30 different classes of adult and pediatric cancers are being subjected PIRL-MS to build a comprehensive molecular signature library using supervised dimensionality reduction and methods. The sensitivity and specificity of the integrated morphometric and molecular diagnosis for pediatric brain cancers with 10-second PIRL-MS was > 96%. This classification could use as little as only 18 tissue lipids whose identities were determined using chromatography and tandem mass spectrometry.

I106

APPROACHES AND STRATEGIES FOR THE DETECTION AND QUANTIFICATION OF NANO – MICROPLASTICS BY SINGLE PARTICLE INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Chady Stephan**, Ruth Merrifield, Liyan Xing and Aaron Hineman. PerkinElmer, Woodbridge, ON, Canada.

Plastic is the most prevalent type of marine debris found in our ocean and lakes. Plastic debris can come in all shapes and sizes, but those that are less than five millimeters in length are called “microplastics.” Microplastics enter the environment from a variety of sources, environment weathering of large plastic items, additive manufacturing used in cosmetics and release from consumer products.

Currently FT-IR microscopy is the most common approach used for microplastic research. Here we show that single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) can be utilized for the analysis of micro- sized plastics by monitoring carbon isotopes. We discuss the use of specific introduction parts, to ensure an even transport efficiency of both dissolved and micron-sized particles into the plasma, as well as strategies using specific gasses and cell conditions to obtain the best detection limits. This approach can be used for fast scanning of microplastic particles in environmental matrices or consumer products without needing to concentrate or alter the samples matrices.

I107

ION DYNAMICS IN LITHIUM and ZINC ION CELLS REVEALED BY MAGNETIC RESONANCE SPECTROSCOPY and RELAXOMETRY.

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Li-ion batteries (LIBs) have become ubiquitous in society, ranging from hand-held portable electronics to widespread adoptions in electric vehicles. Beyond mobile devices, a Net-Zero future requires appropriate energy storage for the grid, for which LIBs are impractical. Alternative chemistries are composed of abundant materials and utilize aqueous electrolytes, which are environmentally friendly, sustainable, and cost-effective. Magnetic resonance spectroscopy and imaging techniques are powerful tools for probing dynamic processes in lithium-ion batteries [1]. We have recently reported the application of a parallel-plate resonator to the *real-time* ^{7}Li *operando* NMR monitoring of Li metal deposition on a graphite anode during repeated charging and discharging of a single layer prismatic cell [2]. The method allows the quantification of the lithiation of the anode material as well as the early detection of plated metallic lithium throughout the duration of cell charging. Optimized ^{1}H and ^{7}Li PPRs are utilized to enable high sensitivity *in situ* and *operando* NMR experiments with fine temporal resolution, allowing identification of transient species such as Mn^{2+}(aq) dissolution, and accumulation of defect sites.

[1] Pecher, O., Carretero-Gonzalez, J., Griffith, K., Grey, C.P., *Chem. Mater.*, 2017, **29** 213−242. DOI.org/10.1021/acs.chemmater.6b03183
[2] K.J. Sanders, J.R. Keffer, A.R. Aguilera, B.J. Balcom, I.C. Halalay, G.R. Goward *Carbon* 2022,**189** (377-385) DOI.org/10.1016/j.carbon.2021.12.082

I108

DEVELOPING REMEDIATION METHODS FOR PFAS IN SOIL AND WATER: ANALYSIS CONSIDERATIONS AND CURRENT PROGRESS.

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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 PFAS soil and water remediation projects at various stages of completion, ranging from lab-scale to field-scale pilots. Projects discussed will include ball-milling, gamma irradiation, UV-activation, combustion, and smouldering combustion. Mechanistic insights and common observations across the suite of remediation techniques, analytical considerations, and the potential paths forward will be discussed.

I109

A NOVEL APPROACH FOR IN SITU DETECTION OF GUNSHOT RESIDUE. **Igor K. Lednev.** University at Albany, State University of New York, 1400 Washington Ave., Albany, NY 12222, USA (ilednev@albany.edu)

Gunshot residue (GSR) is an important type of forensic trace evidence that is produced when a firearm is discharged. GSR can be subdivided into two sub classifications—organic and inorganic. A current method based on scanning electron microscopy coupled with energy dispersive X-ray spectroscopy is used for detection and identification of inorganic GSR particles only. However, the total amount of organic GSR (OGSR) generated due to the discharge of a firearm is much larger than the amount of IGSR. In addition, OGSR particles are typically much larger in size than IGSR particles. We have developed a new two-step approach for fast detection of OGSR particles using fluorescence spectroscopy followed by a confirmatory identification by Raman microspectroscopy. In our first proof-of-concept study we used adhesive tape as a method of collecting OGSR particles. Most recently, we have significantly expanded this methodology by demonstrating the possibility of detecting and identifying GSR particles in situ on cotton fabric eliminating the need for the initial GSR particle transfer stage. In this presentation, we will show the results of these recent studies, discuss challenges and future steps for the proposed two-step method development for the detection and confirmatory identification of GSR.

I110

IDENTIFYING PFAS CHEMICALS IN CONSUMER ANTI-FOG PRODUCT SOLUTIONS USING GC-TOFMS. **Stephan Laperriere**[1], David E. Alonso[2] and Joe Binkley[2], [1]LECO Instruments ULC, 2205 Dunwin Drive, Mississauga, ON, Canada L5L 1X1; [2]LECO Corporation, 3000 Lakeview Avenue, Saint Joseph, Michigan, USA. (stephan_laperriere@leco.com)

Anti-fog solutions are useful for maintaining clean, and clear, protective eyewear for the laboratory, various construction use, and for several sports. Unfortunately, some anti-fog solutions may contain PFAS (Per / Poly-Fluorinated Alkyl Substances), as noted by researchers at Duke University [1]. These organic pollutants in the environment, and so-called “long chain”, and “Forever” chemicals are mobile, persistent and will bioaccumulate. That is, they build up in our bodies, and in other species. They are hazardous, but toxicity has only been investigated thoroughly for a few PFAS. It is important to identify and characterize PFAS and their degradants. To do so, the sample analysis must include Non-Targeted Screening. Now for over more than two decades, LECO has developed a holistic system that combines the strength of several components: multi-introduction system, Gas Chromatography (GC) in one or two dimensions (comprehensive GCxGC), Time-Of-Flight Mass Spectrometry with a Multi-Mode Source (TOFMS with MMS), fast ChromaTOF software, and intricate deconvolution. The objective will be to show how this type of endeavor is crucial to our risk assessment and decision making.

[1] Herkert, Nicholas J., Christopher D. Kassotis, Sharon Zhang, Yuling Han, Vivek Francis Pulikkal, Mei Sun, P Lee Ferguson, and Heather M. Stapleton. Environmental Science & Technology 56, no. 2 (January 2022): 1162–73. https://doi.org/10.1021/acs.est.1c06990.

I111

DETERMINATION OF ATMOSPHERIC PARTICLES USING SINGLE PARTICLE TOF-ICP-MS. Yannick Tardif, Katia Iatariene, Houssame-Eddine Ahabchane, Madjid Hadioui, Patrick Hayes and **Kevin J. Wilkinson,** Biophysical environmental chemistry, University of Montreal, Campus MIL, 1375 Ave. Thérèse-Lavoie-Roux, Montréal, QC, H2V 0B3, Canada.
(kj.wilkinson@umontreal.ca)

Elevated concentrations of fine ($PM_{2.5}$) and ultrafine particulate matter are associated with poor air quality and a variety of adverse health effects. While single particle techniques have the advantage of being able to provide information on the occurrence and nature of low frequency events, such techniques are limited. Single particle inductively coupled plasma time-of-flight mass spectrometry (SP ICP-ToF-MS) was used to compare the composition of aerosol particles collected from pristine, urban and industrial settings. Insight into the limitations due to sampling (collection of particles), analysis (detection limits, multiple dilutions, optimal particle numbers) and data treatment (data filtering, cluster analysis) will be discussed. Particle size detection limits were lowered by using a combination of ion-exchange resins and oversampling. Clustering techniques, based upon elemental composition only, appeared to be the most useful for discriminating samples and identifying markers of atmospheric pollution. Finally, for samples collected from several contrasting sample locations, SP ICP-ToF-MS analysis showed that a detailed analysis of the low frequency events (~<3%) provided more insight into the nature of the sample as opposed to high frequency events that were largely similar among sites.

I112

EXPANSION AND VALIDATION OF A SELF-REFERENCING ALGORITHM TO DISCRIMINATE BETWEEN HUMAN AND ANIMAL BLOOD FOR FORENSIC PURPOSES. **Alexis R. Weber [1],** Harrison Dickler[2], and Igor K. Lednev[2], [1]SupreMEtric LLC; [2]Department of Chemistry, University at Albany, SUNY, 1400 Washington Avenue, Albany, NY 12222, United States. (aweber@albany.edu)

Determining whether a bloodstain is of human or non-human origin is crucial in forensic investigations. In groundbreaking research, Bian et al. introduced a self-reference peak algorithm to analyze the Raman spectra of bloodstains, showcasing its significant potential for distinguishing between human and non-human blood [1]. However, their initial study included only three non-human species in developing the model. The current study enhances this capability by using the self-referencing algorithm to differentiate between human blood and that of 18 non-human species based on Raman spectra. The intensity ratios between the bands at 1003 and 1341 cm^{-1} in the Raman spectra were compared across species to identify a threshold separating human from non-human samples. The algorithm successfully classified spectra averaged from donors of all 18 non-human species. This algorithm is user-friendly, requiring minimal training or statistical knowledge, making it more accessible for forensic use compared to complex computational methods. This Raman spectroscopy technique is rapid, nondestructive, and highly accurate, positioning it as a promising tool for forensic applications.

[1] Bian H., Wang P., Wang J., Yin H., et al. “Discrimination of Human and Nonhuman Blood Using Raman Spectroscopy with Self-Reference Algorithm”. *J. Biomed. Opt*. 2017. 22(9): 1–7.

I113

ELEMENTAL SPECIATION BY OPTICAL EMISSION MICROPLASMA SPECTROMETRY: THE CASE FOR CHROMIUM AND ARSENIC.

Daniel A. Cebula, Liaba Quadeer, V. Zhou, U. Dayal, M. J. W. Thiessen and **Vassili Karanassios**, University of Waterloo, Waterloo, ON, Canada. (vassili.karanassios@uwaterloo.ca)

The determination of the elemental concentration of Chromium species in water samples is of significant importance due to the toxicological effects of the different oxidation states. For example, Cr^{3+} is an essential micronutrient whereas Cr^{6+} is carcinogenic. Similar argument applies to Arsenic species with different oxidation states. In this presentation, speciation of Cr and Arsenic will be discussed in detail. Concentration determinations were accomplished a using a battery-operated microplasma.

I114

ARSENIC SPECIATION IN CHICKEN AND FISH.

Xiufen Lu, Chester Lau, Karen S. Hoy, Tetiana Davydiuk, Haixia Yu, Emma Jing, Kayla LaPorte, Gursevak Uppal, Hanyong Peng, and **X. Chris Le**. Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, University of Alberta, Edmonton, AB T6G 2G3, Canada. (xc.le@ualberta.ca)

Food and water are main sources of human exposure to arsenic. Determination of arsenic speciation in food is important because the toxicity of arsenic varies greatly with its chemical speciation. We report here quantification of arsenic species in chicken meat and freshwater fish. Arsenic species in chicken breast and fish muscle tissue were extracted using water-methanol mixture and with the assistance of sonication and enzyme treatment. Arsenic species in the extracts were separated using high performance liquid chromatography (HPLC) and detected using inductively coupled plasma mass spectrometry (ICPMS). Electrospray ionization tandem mass spectrometry (ESI MS/MS), used in combination with HPLC and ICPMS, provided complementary information for the identification and characterization of arsenic species. A Roxarsone-feeding study, involving 1600 chickens fed either a control diet or the Roxarsone additive for 5 weeks, revealed extensive metabolism of Roxsarsone (a phenylarsonical) in chicken. Analysis of arsenic speciation in more than 1400 freshwater fish samples, representing 14 common fish species from 48 waterbodies in Alberta, showed the presence of arsenobetaine (AsB), dimethylarsinic acid (DMA), and inorganic arsenate (As^V) in almost all samples. Arsenic speciation patterns differed among lake whitefish, northern pike, and walleye, the three most common types of fish collected. An assessment of arsenic intake suggests that moderate consumption of freshwater fish from Alberta waterbodies does not cause significant exposure to toxic arsenic species.

[1] K.S. Hoy, T. Davydiuk, X. Chen, C. Lau, J.R.M. Schofield, X. Lu, J.A. Graydon, R. Mitchell, M. Reichert, X.C. Le, **Food Qual. Safe.** 7 (2023) 1–25.
[2] T. Davydiuk, J. Tao, X. Lu, X.C. Le, *Environ. Health* 1 (2023) 236–248.
[3] H. Peng, B. Hu, Q. Liu, J. Li, X.-F. Li, H.Q. Zhang, X.C. Le, *Angew. Chem. Int. Ed.* 56 (2017) 6773–6777.

I115

ELEMENTAL ANALYSIS IN YEAST CELLS AND MICROPLASTICS BY ICP-MS WITH AUTOMATED MICRO-FLOW SAMPLE INTRODUCTION.

Yan Cheung, Emmett Soffey, and Bastian Georg, Agilent Technologies.

Nanoparticle and Single Cell Elemental Analysis by ICP-MS has become popular in recent years due technological advancements in ICP-MS, as well as increasing needs for applications in various technical areas. On the other hand, microplastics have been the topics of discussions and research as its increasingly important role in environmental applications. Various analytical techniques have their own limitations, such as the ability of particle characterization, particles sizes, and methods of sample introduction. In the current study, an automated, micro-flow autosampler in combination with a triple quadrupole Inductively Coupled Plasma-Mass Spectrometry (ICP-QQQ) is used in the elemental analysis of yeast cells and microplastics. The sample introduction system is designed to deliver intact single cells and microplastics to the plasma, while the ICP-QQQ offers unmatched high sensitivity for elemental determination within the cells and microplastics. Preliminary laboratory experiments in single cell study showed the potential of applying the sample introduction setup to other single cell applications, while the preliminary results from microplastics study showed ICP-QQQ can be good complimentary technique to other analytical techniques for microplastics (such as LDIR). Microplastics with sizes down to 1 micron in aqueous solution were detected and analyzed by ICP-QQQ.

I116

COMPARING SAMPLE PREPARATION STRATEGIES FOR THE DETERMINATION OF MAJOR COMPONENTS IN BLACK MASS WITH THE AVIO® 550 MAX ICP-OES.

Ken Neubauer, **Aaron Hineman**, PerkinElmer, 710 Bridgeport Ave, Shelton, CT, 06484, USA.
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With the growing adoption and use of lithium-ion batteries, the need to increase production has also risen. A major challenge of increasing production is acquiring the necessary raw materials, particularly elements common in cathode materials, and while these elements can be extracted from the earth, expanding mining operations has a large negative environmental impact. One way to minimize the negative environmental impact of lithium-ion battery production is through recycling by recovering important metals from spent batteries and using them to make new ones. One of the most common recycling methods involves shredding and incineration of batteries, which results in “black mass” – a mixture of metals, ash, graphite, and residual electrolyte – which must be analyzed both for elements of interest (primarily cathode elements) as well as other high-level contaminants. Because of the complex nature of black mass and the concentrations of interest, ICP-OES is the technique of choice for the analysis, however, a major analytical challenge involves sample preparation: since ICP-OES can only analyze samples in liquid form, the black mass must be converted to a liquid for analysis. With the amounts of ash and graphite present, this poses a challenge. This work compares sample preparation methods for battery recycling black mass (aqua regia leaching, microwave digestion, and lithium and sodium fusions), with analysis using the Avio® 550 Max ICP-OES. Each sample preparation strategy has advantages and limitations, both in execution and considering the elements measured. The Avio 550 Max fully simultaneous ICP-OES easily performs measurements from each sample preparation methodology and provides initial sample screening through SmartQuant™, allowing users to determine which elements may be present in various concentration ranges.

I117 P

BIS(2-ETHYLHEXYL)-2,3,4,5-TETRABROMOPHTHALATE ENHANCES *FOXO1*-MEDIATED LIPOPHAGY TO REMODEL LIPID METABOLISM IN ZEBRAFISH LIVER.

Jian Han, University of Alberta, Division of Analytical and Environmental Toxicology, Edmonton, AB T6G 2G3, Canada. (jhan23@ualberta.ca)

An emerging environmental contaminant, bis(2-ethylhexyl)-2,3,4,5-tetrabromophthalate (TBPH), can bioaccumulate in the liver and affect hepatic lipid metabolism. However, the in-depth mechanism has yet to be comprehensively explored. In this study, we utilized transgenic zebrafish Tg (*Apo14: GFP*) to image the interference of TBPH on zebrafish liver development and lipid metabolism at the early development stage. Using integrated lipidomic and transcriptomic analyses to profile the lipid remodeling effect, we uncovered the potential effects of TBPH on lipophagy-related signaling pathways in zebrafish larvae. Decreased lipid contents accompanied by enhanced lipophagy were confirmed by the measurements of Oil Red O staining and transmission electron microscopy in liver tissues. Particularly, the regulatory role of the *foxo1* factor was validated via its transcriptional inhibitor. Double immunofluorescence staining integrated with biochemical analysis indicated that the enhanced lipophagy and mitochondrial fatty acid oxidation induced by TBPH were reversed by the *foxo1* inhibitor. To summarize, our study reveals, for the first time, the essential role of *foxo1*-mediated lipophagy in TBPH-induced lipid metabolic disorders and hepatoxicity, providing new insights for metabolic disease studies and ecological health risk assessment of TBPH.

I118 P

DETECTION OF SARS-COV-2 RNA IN NASOPHARYNGEAL SWAB AND SALIVA USING AN RNA-BRIDGED DNA HYDROGEL CAPILLARY SENSOR.

Honghong Wang, X. Chris Le, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, University of Alberta, Edmonton, Alberta, T6G 2G3, Canada. (honghon2@ualberta.ca)

Rapid and sensitive detection of specific nucleic acid sequences of infectious agents is critical for diagnosis of infectious diseases and community surveillance. The objective of this research was to apply a newly developed point-of-care technique to the determination of severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) RNA. The viral RNA was extracted from nasopharyngeal swab and saliva samples. The viral RNA was detected using an RNA-bridged DNA hydrogel capillary sensor, a technique we developed for the detection of specific RNA sequences. Results from the analysis of 17 nasopharyngeal swab samples and 10 saliva samples were in agreement with the results of the standard polymerase chain reaction (PCR) analysis. Integration of the CRISPR/Cas13a into the RNA-bridged DNA hydrogel facilitated recognition of the specific RNA sequence and increased the detection specificity. This technique provided visual detection with the naked eyes, without the need for any photoelectric equipment for detection. Quantification was achieved by measuring distances using a ruler. This technique has great potential for point-of-care, onsite, and at-home applications.

I119 P

CHEMICAL CONTAMINANTS IN TRADITION FOODS: BEFORE AND AFTER THE WILDFIRES. **Xiufen Lu**[1] and X. Chris Le[1,2], [1]Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, University of Alberta, Alberta T6G 2G3, Canada; [2]Department of Chemistry, Faculty of Science, University of Alberta, Edmonton, AB, T6G 2G2, Canada. (xlu@ualberta.ca)

On May 1, 2016, a wildfire began southwest of Fort McMurray, Alberta, and the wildfire destroyed more than 2000 homes and buildings. Burning of the CCA treated wood resulted in the release of arsenic, copper, and chromium to the environment. There were substantial concerns over the effect of wildfires on air, water, and food quality. To address the concern of potential effect of the wildfires on local food, our study focused on the determination of metals and metalloids in local food. we analyzed fish, berry, and vegetable samples collected from Fort McMurray and Farmers Market Edmonton in 2014, 2015, 2016, 2017 and 2018. Inductively coupled plasma mass spectrometry (ICPMS) was used for the analysis. There was no significant difference in the arsenic concentrations between fish samples collected before and after the wildfires. We also compared the arsenic concentrations between fish samples collected from northern Alberta and from other Lakes in Alberta, and berry samples collected in 2014, 2015, 2016 and 2017 with vegetable samples purchased from Edmonton farmers markets. There was no significant difference. These results suggest that concentrations of arsenic in local fish and berries were not increased by the wildfires of 2016.

I120 P

CRISPR/CAS13A-RESPONSIVE AND RNA-BRIDGEED DNA HYDROGEL CAPILLARY SENSOR FOR POINT-OF-CARE DETECTION OF RNA. **Hui Wang**, Honghong Wang and X. Chris Le. University of Alberta, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, Edmonton, Alberta, T6G 2G3, Canada (hui19@ualberta.ca)

Point-of-care (POC) tests can complement centralized laboratory analysis and meet increasing needs for diagnostics and surveillance, especially in resource-limited settings and remote areas. The objective of this research was to develop a POC assay without the need for optical or electrical equipment. We developed a CRISPR/Cas13a-responsive and RNA-bridged DNA hydrogel capillary sensor for the direct and visual detection of specific RNA with high sensitivity. The capillary sensor was simply prepared by loading RNA-crosslinking DNA hydrogel film at the end of a capillary. When the CRISPR/Cas13a specifically recognized the target RNA, the RNA bridge in the hydrogel film was cleaved by the *trans*-cleavage activity of CRISPR/Cas13a, increasing the permeability of the hydrogel film. Different concentrations of target RNA activated different amounts of Cas13a, cleaving different amounts of the RNA bridge in the hydrogel and causing corresponding changes in the permeability of the hydrogel. Therefore, samples containing different amounts of the target RNA traveled to different distances in the capillary. Visual reading of the distance provided quantitative detection of the RNA target without the need for any nucleic acid amplification or auxiliary equipment.

I121

END-TO-END AUTOMATED HIGH THROUGHPUT CHEMICAL ANALYSIS OF TIRE DERIVED PARA-PHENYLENE DIAMINE QUINONES (PPDQs) USING ONLINE MEMBRANE INTRODUCTION ESI-MS/MS. Joseph Monaghan, Angelina Jaeger, Chris G. Gill, **Erik T. Krogh**, Applied Environmental Research Laboratories, Department of Chemistry, Vancouver Island University, 900 Fifth Street, Nanaimo, British Columbia, Canada; Department of Chemistry, University of Victoria, PO Box 3055, Victoria, British Columbia, Canada. (erik.krogh@viu.ca)

Phenylene diamine quinones leached from tire wear particles have been shown to be acutely toxic to salmonids and associated with urban run-off mortality syndrome in the Pacific Northwest [1]. Given the ubiquity of these contaminants in urban waterways, we developed a high throughput analytical workflow to enable wide scale surveillance to characterize their fate and distribution. We discuss recent advances and analytical performance metrics for a direct mass spectrometry approach using a semi-permeable polydimethylsiloxane membrane, providing a '*fit-for-purpose*' method for analysis in storm and surface waters with an analytical duty cycle of < 4 min/sample and limits of detection < 10 ng/L [2]. Combining a purpose-built smartphone sample collection app, low-cost auto-sampler, and data processing tools provides end-to-end automation enabling rapid reporting and adaptive sampling. We will present results from a large citizen science sampling campaign (> 2000 samples) on Vancouver Island (BC, Canada) from Fall 2023 including targeted high intensity spatiotemporal sampling. Working with project partners, we leverage this high throughput analysis platform to investigate environmental exposures, inform risk assessments, and prioritize mitigation practices.

[1] Tian et al., *Science* **2021,** 371, 185−189. DOI : 10.1126/science.abd6951
[2] Monaghan et al., *ACS ES&T Water* **2023** *3* (10), 3293-3304 DOI: 10.1021/acsestwater.3c00275

I122

OVERVIEW OF A “TOTAL WORKFLOW” APPROACH TO SAMPLE PREPARATION AND WHY IT MATTERS. **Geoff Williams** and Luca Bertoli, ATS Scientific, Burlington, ON, Canada.

The 'total workflow' approach to sample preparation for elemental analysis examines not only the evolution of the microwave digestion process, but also other workflow steps that are critical to meeting laboratory performance requirements. By optimizing these steps, laboratories are better prepared to overcome the challenges they face and avoid workflow disruptions that impede the analysis process and can have additional effects.

I123

HIGH ENTROPY ALLOYS FOR ELECTROCHEMICAL BIOSENSING APPLICATIONS

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The electrochemical detection of bioanalytical compounds by redox reactions typically has a complex pathway with multiple steps and intermediates involved. As research is being conducted to develop non-enzymatic electrochemical sensors based on inorganic catalyst, new avenues are being explored to improve sensitivity and selectivity which are a challenge. In this aspect high entropy alloys (HEAs) that are composed of five or more elements and as a result are stabilized by configurational entropy are a promising avenue. Due to elemental heterogeneity, their surface has multiple active sites which can catalyze different steps in a reaction pathway, while maintaining stability due to thermodynamics. The millions of possible elemental combinations for HEAs present an opportunity to tailor them as high performance electrocatalyst. Here we briefly present the formation of such multi-element composites for detection of Lactate and its comparison to traditional single element and bi-elemental compositions. The synthesis process and characterization results will be discussed to show the compositional heterogeneity of the material. Then its electrochemical performance will be discussed.

I124

ANALYTICAL SOLUTIONS FOR THE LITHIUM-ION BATTERY VALUE CHAIN.

Bernd Bletzinger, Nora Engel, and Florian Schuart. Analytik Jena. Presenter: **Bartosz Jasiak**

The production of high-quality lithium-ion batteries entails a complex process spanning resource extraction, material refinement, production, and recycling, necessitating meticulous element analysis throughout. This paper explores the challenges and solutions pertaining to elemental analysis in each phase of the value chain, from mining to recycling, in order to ensure optimal quality and safety. Battery manufacturers monitor raw material contaminants to guarantee product quality, while recycling facilities verify material purity and comply with environmental regulations. This article highlights the efforts of companies like Analytik Jena, collaborating with the industry, to develop high-quality valuable products based on scientific insights and optimal methodologies, with robust and sensitive analytics as a cornerstone. The upstream process is explored first, addressing ore exploration and refinement. Eighty percent of a Li-ion battery's value is determined by its constituent materials, emphasizing the need for premium-quality resources. China currently dominates both raw material extraction and battery production, with the European market largely relying on imports. However, the discovery of lithium deposits in other regions offers potential for increased production independence. The extraction of key materials for lithium-ion batteries involves complex processes. This paper discusses different aspects of quantifying these elements in various phases of the battery life cycle, touching on sample preparation and spectroscopic techniques for element analysis. Furthermore, the monitoring of wastewater from the battery production process using various analytical techniques to comply with environmental regulations is addressed. In conclusion, the critical role of analytical techniques in ensuring the quality and environmental responsibility of lithium-ion battery production is discussed.

I125 P

CONTINUOUS ON-LINE LEACHING BIO-ACCESSIBILITY STUDIES OF BLACK SOLDIER FLY LARVAE USING INDUCTIVELY COUPLD PLASMA MASS SPECTROMETRY.

Qiqi Zhang[1], Zoltan Mester[2], Diane Beauchemin[1], [1]Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada; [2]National Research Council of Canada, Metrology Research Centre, 1200 Montreal Rd, Ottawa, ON K1A 0R6, Canada. (17qz@queensu.ca)

Black soldier fly larvae, as the most sustainable alternative protein sources among all edible insects, have been studied extensively for use as waste management and animal feed. As little is known about their use as human food, the previously established continuous on-line leaching method (COLM) coupled with inductively coupled plasma mass spectrometry (ICPMS) has been applied to measure their bio-accessible metal(loid)s concentrations of As, Cr, Se, Cd, Pb, and Ni. However, the usage of stainless-steel column has been found to induce clogging and leaching of column contained elements. Here we showed that replacing the metal column with a polypropylene flash column generates better results. This transparent column enables visualization of the digestion processes and reduces column background and back pressure. The modified COLM ensures quick risk assessment and isotopic source identification. Following the Guidance on Human Health Preliminary Quantitative Risk Assessment (PQRA), BSFL are safe to consume for all ages (except for infants) if people keep their regular daily protein intake and consume BSFL 2 days per week, except for the carcinogenic risk of arsenic. Speciation analysis of the bio-accessible As fraction is necessary to ensure the safe human consumption of BSFL.

I126

ENHANCING SINGLE PARTICLE ICPMS PERFORMANCE WITH AN OPTIMIZED INFRARED HEATED SAMPLE INTRODUCTION SYSTEM FOR TOTAL CONSUMPTION,

Zichao Zhou[1], Mirah J. Burgener[2], John Burgener[2] and Diane Beauchemin[1], [1]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; [2]Burgener Research Inc, Canada. (16zz39@queensu.ca)

Single particle inductively coupled plasma mass spectrometry (spICPMS) is a powerful technique for characterizing nanoparticles (NPs). However, its sensitivity and detection limits are restricted by the low transport efficiency of conventional sample introduction systems [1]. This work aimed to optimize an infrared (IR) heated sample introduction system on a NexION 2000 ICPMS instrument to achieve total sample consumption and improve the size detection limit for NPs. Eight modified cyclonic spray chambers with volumes ranging from 25 to 125 mL, with an IR emitter inserted in a modified baffle and varying gaps between the baffle top and the spray chamber top, are tested to evaluate their effect on sensitivity, detection limit, and transport efficiency for NPs characterization. A multivariate optimization of IR heating temperature, sample uptake rate, nebulizer gas flow rate, and sampling depth was performed. The results indicate that the 50-2mm modified spray chamber offers the best performance in terms of detection limit, enhancing sensitivity and precision of Au and MC 25-2mm works best for Pt. These spray chambers were selected for characterizing Au and Pt NPs.

I127

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

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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. Additionally, the effect of different spray chamber designs was observed when utilizing IR heating. This research will benefit the analytical services industry by enhancing mineral analysis results while cutting waste disposal costs.

[1] A. Al Hejami, M. J. Burgener, J. Burgener, D. Beauchemin, *J. Anal. At. Spectrom.* 35 (**2020**) 1450-1454.

I128

EXPLORING THE CAPABILITIES OF LIBS AND LA-ICP-MS FOR HIGH-SPEED IMAGING.

C Derrick Quarles Jr.,[1] Benjamin T. Manard,[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-ICP-MS) has become an intriguing option for elemental imaging. This technique offers high-speed (≥1000 Hz), highly-spatial (nm to µm) information with excellent detection limits (sub-ppb to ppb). The only negative for ICP-MS is that it utilizes an atmospheric plasma generated by argon gas, therefore, atmospheric elements (H, N, O) and F (ionization potential is higher than that of Ar) are not accessible. Laser-induced breakdown spectroscopy (LIBS), when operated in a helium purged atmosphere can excite and detect H, N, O, and F, in addition to all other elements on the periodic table. Thus, combining LIBS and LA-ICP-MS provides elemental coverage for the entire periodic table. In this work, an 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). This presentation will go over how this combined LIBS and LA-ICP-MS technology works, in addition to going into applications that cover the geochemistry, battery, nuclear materials, and life science areas.

I129

VALIDATION OF A GREENER METHOD OF SEX DETERMINATION THROUGH THE MULTI-ELEMENTAL ANALYSIS OF HAIR USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY.

Chloe Wheeler and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (18clw1@queensu.ca)

In forensic applications, head hair serves as a reliable biomarker since it contains a permanent record of elements from an individual's body. By substituting CF_4 reaction gas for polytetrafluoroethylene (PTFE) powder, this research modifies and re-optimizes a previous method [1] for determining the sex of humans by directly analyzing hair samples via electrothermal vaporization inductively coupled plasma optical emission spectrometry (ETV-ICPOES). Similarly, this method uses an Ar emission line to compensate for sample loading effects on the plasma via point-by-point internal standardization. Then, background correction and peak area integration are performed, followed by multivariate analysis, including principal component analysis (PCA) and linear discriminant analysis (LDA) in which Mg, S, Sr, and Zn concentrations are used to accurately predict the sex of male and female samples. In future research, this method will be expanded to include dyed hair, and hair from people of different races and ethnicities, which will significantly increase its robustness. Ultimately, this research offers an alternative model that employs green chemistry and uses a more affordable and accessible carrier agent at no cost to the original method's reliability.

[1] M. MacConnachie, S. Lu, Y. Wang, J. Williams, D. Beauchemin, *RSC Adv.* 12 (**2022**) 27064-27071.

I130

STATE-OF-THE-ART ICPMS SAMPLE INTRODUCTION SYSTEMS FOR NANOPARTICLE, SINGLE CELL, AND ELEMENTAL SPECIATION.

C Derrick Quarles Jr.,[1] Patrick Sullivan,[2] Benjamin T. Manard,[2] Paula Menero Valdes,[3] Beatriz Fernandez[3], [1]Elemental Scientific, Inc., Omaha, NE, USA ; [2]Oak Ridge National Laboratory, Oak Ridge, TN, USA; [3]University of Oviedo, Oviedo, Spain. (Derrick.Quarles@icpms.com)

Inductively coupled plasma mass spectrometry (ICPMS) has become the workhorse instrumentation for elemental analysis. The flexibility of the ICPMS to be coupled with various sample introduction systems has allowed for many techniques to emerge, such as liquid chromatography (LC)-ICPMS, laser ablation (LA)-ICPMS, single particle (sp)-ICPMS, and single cell (sc)-ICPMS. This work will focus on automating these techniques, specifically LC-ICPMS, sp-ICPMS, and sc-ICPMS, but also keeping them flexible enough to be able to run routine samples without massive instrumental changes. To demonstrate the performance, results from urine As speciation (LC-ICPMS), Au and Pt nanoparticles (sp-ICPMS), and ARPE-19 cells (sc-ICPMS) will be presented.

I131

DEVELOPMENT OF A DIRECT ANALYSIS METHOD TO INFER SEX FROM CHILD HEAD HAIR USING ETV-ICPOES.

Darrian Prendergast, Yangyang Wang and Diane Beauchemin. Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada. (diane.beauchemin@queensu.ca)

Sex determination of children's remains is hindered by the limited number of available techniques which can be poorly established, controversial, or primarily applied to adults. Previous works used multi-elemental analysis of human head hair to infer sex in adults [1] and mummified individuals [2]. Additional work expanded the head hair project to determine the influence of chemical dyes and the impact of including so-called 'nuclear family' on the preliminary model [3]. This research aims to further extend this approach to the analysis of children's hair samples in effort to address an existing gap in the identification of children's remains. All hair samples were washed with doubly deionized water, dried, and ground into a fine powder. Multi-elemental analysis was conducted using electrothermal vaporization (ETV) coupled to inductively coupled optical emission spectrometry (ICPOES). Point-by-point internal standardization using the Ar 404.442 nm emission line was followed by blank subtraction, peak area integration, and mass correction. Principal component analysis (PCA) and linear discriminant analysis (LDA) were used as dimension reducing techniques to identify elements acting as key differentiators of sex. Using Zn, Sr, S, Cu and Ni as predictor elements, all samples were correctly predicted as being male or female regardless of the individual being an adult or a child. These results demonstrate an initial step towards the development of a method for sex determination that can be reliably applied to the analysis of children's and adult's remains.

[1] L. Huang, D. Beauchemin, *J. Anal. At. Spectrom*. 29 (2014) 1228–1232.
[2] M. MacConnachie et al. *RSC Adv*. 12 (2022) 27064–27071.
[3] M. MacConnachie, D. Beauchemin, *J. Anal. At. Spectrom*. 28 (2023) 1394-1401.

I132

OPTIMIZATION OF A METHOD FOR THE PRECONCENTRATION OF NOBLE METALS ANALYZED BY INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY WITH FLOW INJECTION.

Madison Langley, Sarah Meston, Diane Beauchemin. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston ON K7l 3N6, Canada. (19mel1@queensu.ca)

Analytical boundaries are present in the determination of noble metals in environmental samples such as their occurrence at low concentrations and complex matrices. One batch method involved alumina as a sorbent for the selective adsorption of chloro-complexes of noble metals Ru, Rh, Pd, Re, Os, Ir, Pt, and Ag using 2 M HCl. Unfortunately, different eluents had to be used to recover different elements prior to analysis by inductively coupled plasma mass spectrometry (ICPMS) and the method did not include Au. Thiourea was needed to recover Au but was avoided in the eluent because it induced drift. In this work, flow injection (FI) was used to prevent drift and thus enable the use of thiourea so as to allow a single elution. The samples were eluted with a mixture of thiourea and aqua regia and then analyzed using FI-ICPMS. The effect of various parameters, including eluent, sorbent pH, and column wash was studied to find conditions to provide a 25-fold preconcentration for all the noble metals in a single elution from one sample aliquot.

I133

MODIFIED SYNTHETIC PRECIPITATION LEACHING PROCEDURE (MSPLP) FOR ASSESSING THE MOBILITY OF ORGANIC AND METALLIC CONTAMINANTS FROM LAND APPLICATION OF RELOCATED SOILS IN ONTARIO. **Taddese Godeto**,[1] Chunyan Hao,[1] Peter Drouin,[1] Ralph Ruffolo, and Andrew McDonough[2], [1]Laboratory Services Branch and [2]Environmental Monitoring and Reporting Branch, Ministry of the Environment, Conservation and Parks (MECP), 125 Resources Road, Toronto, ON M9P 3V6, Canada. (Taddese.Godeto@ontario.ca)

Excess soil is soil that has been dug up, typically during construction activities, that must be relocated or moved off-site (e.g., natural areas, agricultural lands). About 25 million m^3 of excess soil is generated in Ontario every year. To ensure the proper management of excess soils and reduce impacts to ground or surface water quality in the receiving site, the province has developed an excess soil regulation (O. Reg. 406/19), which incorporates risk-based standards for contaminants that require leachate analysis to determine potential impacts on reuse sites. The Synthetic Precipitation Leaching Procedure (SPLP) developed by the US EPA is one approach used to assess the mobility to water bodies of organic and inorganic contaminants in soils leached under slightly acidic rainfall conditions. The Ministry of the Environment, Conservation and Parks laboratory developed a variation of the SPLP adopting the average rainfall pH in Ontario in batch tests in which contaminants are partitioned between soil solids and an extracting fluid (20:1 ratio of fluid to solid). This study reports the details of the modified leaching procedure and the levels of regulated contaminants in Ontario assessed in leachates of representative background soils (18 metals, 28 organic compounds).

I134

ANALYSIS OF NUTRITIONAL ELEMENTS IN YELLOWKNIFE GARDEN VEGETABLES. **Andre Castillo**[1], Diane Beauchemin[1], Iris Koch[2], Mike Palmer[3], [1]Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; [2]Environmental Sciences Group, Royal Military College of Canada, Kingston, ON, CA K7K 7B4, Canada; [3]North Slave Research Centre, Aurora Research Institute, Aurora College, Yellowknife, NWT, CA X1A 2R3, Canada. (12aic1@queensu.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, but as part of the study, data was collected on concentrations of essential nutritional elements in residential garden soils and vegetables. This allows the consideration of the benefits of consuming garden vegetables, since essential nutrients such as Ca, Fe, K and Zn are important for maintaining good health, and the consumption of vegetables are essential part of a healthy diet. The results of the study will present total concentrations of nutritional elements and bioaccumulation/transfer factors (TFs) in various types of garden vegetables from Yellowknife, and comparisons to baseline nutritional elemental content in vegetables obtained from online sources.

I135

EMERGING DRINKING WATER DISINFECTION BYPRODUCTS: ANALYTICAL AND TOXICOLOGICAL RESEARCH. Qiming Shen, K.N. Minh Chau, Emma Jing, and **Xing-Fang Li**, Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, University of Alberta, Edmonton, Alberta. (xingfang.li@ualberta.ca)

Appropriate disinfection of drinking water is effective to prevent waterborne disease. An unintended consequence of the chemical disinfection process is the formation of disinfection byproducts (DBPs), resulting from reactions of disinfectants with organic matter in source water. Epidemiological studies have indicated potential association of chronic DBP exposure with adverse health effects (e.g. increased risk of bladder cancer). Although a few easily detectable DBPs are regulated, they may not be responsible for the adverse health effects. To meet growing water demands while controlling regulated DBP formation, water utilities are applying new disinfectant combinations. In light of these changes in disinfection practice, we must characterize DBPs that are important to human health effects. This presentation will describe our current research on identifying new DBPs of toxicological importance and their precursors using targeted and nontargeted approaches, understanding the formation of new DBPs, and characterizing toxicity of the identified new DBPs.

I136

ACCURATE ULTRA-TRACE MEASUREMENTS OF ^{236}U USING THE NEXION 5000 ICP-MS. Liyan Xing[1], Karl Andreas Jensen[2], Chady Stephan[1], and Aaron Hinemann[1], [1]PerkinElmer U.S. LLC; [2]Norwegian University of Life Sciences. (Liyan.Xing@perkinelmer.com)

U-236 is the product of thermal neutron capture of ^{235}U, but the natural occurrence of ^{236}U is very rare. The presence of this isotope indicates a nuclear reactor origin of the sample.

ICP-MS is becoming the technique of choice for the measurement of long-lived radionuclides due to its affordability and ease of use compared to other techniques. However, accurate ultra trace-level analysis of the ^{236}U/^{238}U using ICP-MS requires proper interference management. The measurement of ^{236}U$^+$ is subject to interference by peak tailing from the adjacent ^{235}U$^+$ peak and its hydride species ^{235}U^{1}H$^+$.

The NexION® 5000 multi-quadrupole ICP-MS is equipped with two full-length quadrupole mass analyzers ensuring that a typical < 0.7 amu mass resolution can be achieved for both analyzers, while keeping high transmission efficiency. For the analysis of ^{236}U in Mass Shift mode, only ^{236}U$^+$ and ^{235}U^{1}H$^+$ are selected in the first analyzer quadruple and transmitted to the Universal Cell (Q2), while ^{235}U is rejected, and therefore, will not interfere with the downstream reaction and analysis.

I137

NMR AT ULTRA HIGH MAGNETIC FIELD: OPPORTUNITIES AND CHALLENGES FOR BIOLOGICAL AND MATERIALS SOLIDS.

Chad M. Rienstra, University of Wisconsin-Madison, Department of Biochemistry and National Magnetic Resonance Facility at Madison (NMRFAM), 433 Babcock Dr., Madison, WI 53706, United States. (crienstra@wisc.edu)

In this lecture, I will describe the recently upgraded capabilities for solid-state NMR (SSNMR) at NMRFAM, including the first GHz-class magnet in North America dedicated to SSNMR. Since 2020, we have installed and/or upgraded 7 spectrometers (3 600 MHz, 2 750 MHz, 900 MHz, and 1.1 GHz) with custom magic-angle spinning probes designed for biological and materials solids applications. The custom probes include: Varian/Phoenix compatible 1.2 mm, 1.6 mm, 2.5 mm, 3.2 mm and 5.0 mm probes with broadband capabilities (HFXY including low-gamma option); and Black Fox probes with 1.6 mm (900 MHz and 1.1 GHz) and 2.5 mm (900 MHz) Phoenix stators, optimized for low E field and high ^{13}C detection sensitivity. I will highlight applications from my own research group, including structural studies of alpha-synuclein fibrils and the antifungal drug amphotericin B, as well as collaborative user projects at NMRFAM ranging from materials solids to high molecular weight proteins. The NMRFAM user facility is supported by U.S. National Institutes of Health (NIH) R24GM141526, technology development by NIH P41GM136463, and the 1.1 GHz installation is part of the Network for Advanced NMR (NAN) funded by the U.S. National Science Foundation (NSF) Mid-Scale Research Infrastructure grant number 1946970.

I138

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.

I139

WHY AND WHERE IS THERE ARSENIC IN SIFTON BOG? METAL CONTAMINANTS IN SOUTHERN ONTARIO PEAT BOGS.

Helen Lord,[1] Iris Koch[2] and Diane Beauchemin[1], [1]Queen's University, Department of Chemistry, Kingston, ON, K7L 3N7, Canada; [2]Royal Military College of Canada, Kingston, ON, K7K ZB4, Canada. (17hgl1@queensu.ca)

Southern Ontario soils have been used in agricultural production for over 150 years[1] with accompanying concerns regarding metal additions in the soils from historical fertilizer or pesticide use. Prevalent pesticides in Ontario have included calcium and lead arsenate, used for orchards.[1] Sifton Bog is a peatland located in London, Ontario, located near a site recorded as having been used as an orchard; [2] peatlands are of interest when considering arsenic transformations, as the generally anoxic, waterlogged, and organic conditions can impact the As species present [3] . Preliminary sampling of Sifton Bog displayed As concentrations up to 30 mg/kg. To further evaluate this area, which functions as an urban parkland, 22 samples from 9 different locations and various depths were collected. Total As concentrations were analyzed in the samples using inductively coupled plasma mass spectrometry (ICPMS) and reported As concentrations are lower than in the preliminary samples, with the highest concentration being 6.7 mg/kg. In future work, the As speciation will be investigated, along with other contaminants associated with urban impacts, such as Pb and PFAS.

I140

SURFACE-ENHANCED RAMAN SCATTERING (SERS) APPLICATIONS, QUANTIFICATION AND SINGLE MOLECULE SPECTROSCOPY.

Alexandre G. Brolo, University of Victoria, Department of Chemistry, 3800 Finnerty Road, Victoria BC V8P 5C2, Canada. (agbrolo@uvic.ca)

Surface-enhanced Raman scattering (SERS) is a highly sensitive spectroscopy method [1]. In this presentation, we will discuss examples of application of SERS in biomedicine. These include the application of SERS in immunoassays to identify infectious diseases [2] and to identify metabolites from cancer cells subjected to radiotherapy. In certain conditions, the SERS efficiency cross section rival that of fluorescence emissions, allowing the observation of events assigned to single molecules. We will discuss strong fluctuations in SERS intensities that can be assigned from single molecules molecules adsorbed on single nanoparticles [3]. The super-localization of these fluctuations provide some insights into the nature of the nanoenvironment in a SERS system. Finally, we will discuss approaches for quantification in SERS at ultra-low concentrations. Particularly, we will review that factors that affect SERS quantification and demonstrate a digital approach that allow quantification of model environmental contaminants at very low levels [4].

[1] M. Fan, G.F.S, Andrade, AG Brolo, Anal. Chim. Acta, 693 (2011) 7-25
[2] A. T. Bido, A. Azarakhshi, A.G. Brolo, Anal. Chem., 94 (2022) 17031-17038
[3] N. C. Lindquist and A. G. Brolo, J. Phys. Chem., 125 (2021), 7523-7532
[4] C.D.L. de Albuquerque, R.G. Sobral-Filho, R.J. Poppi, A.G. Brolo, Anal. Chem., 90 (2018) 1248-1254

I141

SNRG BLOCK SYSTEM: THE MOST VERSATILE ACID DIGESTION BLOCK FOR METALS ANALYSIS. **Rachid Choudar**, Analytichem, 21800 Clark Graham, Baie d'Urfé, QC H9X 4B6, Canada.

The SNRG Block™ system offers an innovative design and high temperature uniformity, providing a reliable sample digestion system suitable for methods up to 240°C.

Designed for flexibility, the SNRG Block™ adapts to your laboratory workflow, delivering reliable performance and better control over the acid digestion process. It supports different sized tubes from 15ml to 100ml, allowing for high-throughput processing, all on one system, using different sized graphite inserts.

The large 7" touch screen is easy to navigate and features a built-in magnet for mounting or a kickstand for tabletop placement. It allows you to create multi-step methods, track digestion progress in real-time, and store up to 60 files. The system enables the storage of methods such as "Time to Temperature" and "Time at Temperature." Users can also save detailed reports onto a USB stick for laboratory audits.

With the SNRG Block™ integrated into your lab workflow, you can trust your data and use resources efficiently. Achieving lasting synergy in the lab involves pairing optimal sample preparation with instrumental analysis and implementing robust control through reference materials.

I142

TOWARD A MINIATURIZED INSTRUMENT FOR DETERMINATIONS USING QUANTUM DOTS AND SELECTED ENVIRONMENTAL SAMPLES. **Vassili Karanassios**, U. Dayal and M. J. W. Thiessen, University of Waterloo, Waterloo, ON, Canada.

Quantum Dots (QDs) have been receiving significant attention due to their scientific interest (e.g., they were awarded the Nobel Prize in Chemistry in 2023) and their technological applications (e.g., television displays). In this paper, the application of Quantum Dots (primarily) for detection of metal ions in water samples or in biological samples (e.g., blood syrum) will be described in some detail and future directions will be discussed.

I143

ARTIFICIAL INTELLIGENCE (AI) APPLICATIONS: FROM MATERIAL ANALYSIS USING MICROPLASMAS TO AI DRIVEN MATERIALS SYNTHESIS. **Terje Nissen Farup** and Vassili Karanassios, University of Waterloo, Waterloo, ON, Canada.

For use on-site for sample analysis, optical emission spectrometers must become portable and hence smaller. However, as spectrometers become smaller, their focal length must decrease. But as their focal length decreases, spectral overlaps become an issue that must be addressed. In the first part of this presentation, spectral interference correction using AI (in the form of Artificial Neural Networks or ANNs) will be described. In the second part, AI-assisted (e.g., using generative AI) development of new materials with designer, tailor-made properties will be described. As well, in this part, a brief technical introduction to AI and how we're using it aiding discovery of new materials will be described.

I144

MULTIPLEXED IMAGING OF LIVE BIOLOGICAL SYSTEM: SEEKING OPPORTUNITIES FOR MINIATURIZED SPECTROSCOPIC IMAGING PLATFORMS.

Jung-Ho Yu, University of Waterloo, Waterloo, ON, Canada.

In this talk, I will present our chemistry efforts to develop an *in vivo* multiplexed imaging method of live mouse models and its potential clinical translation. On the extension of this technology, I am seeking opportunities to miniaturize the multiplexed imaging platform for more diverse applications.

- Multiplexed Imaging of Tumor Xenograft Live Mouse Models [1]. We have utilized the high spectral resolution of SERS signals for *in vivo* multiplexed imaging of tumor xenograft mouse models. To gain sufficient brightness for the *in vivo* imaging condition, we controlled SERS nanoparticles oligomerization to produce multicore SERS nanoparticles, which displayed Raman scattering as bright as near-infrared (NIR) fluorescence. The large enhancement factor from hot-spot geometry of the multicore nanoparticles, along with the NIR-resonant Raman reporters, produced the SERS signals as bright as NIR fluorescence. With the multicore SERS nanoparticle palettes, we demonstrated noninvasive and five-plex ratiometric imaging of tumors in live preclinical models, which simulated the noninvasive assessment of multiple biological targets within tumors.
- *In Vivo* Excretable Supramolecular Raman Nanoparticles [2]. While the colloidal SERS nanoparticles have limited their use in humans because of their inability to excrete from the body, we address this problem by creating supraparticles composed of small-sized nanoclusters. We performed the FDTD simulation of the supraparticle design, in which the maximum enhancement factor of 106 was achieved. Then, we chemically synthesized bright supraparticles that enabled *in vivo* Raman imaging of live mouse models. Furthermore, the supraparticles were highly excretable, offering great potential for translational application of the surface-enhanced Raman scattering imaging by replacing non-excretable SERS nanotags.

[1] Yu JH *et al*. Noninvasive and Highly Multiplexed Five-Color Tumor Imaging of Multicore Near-Infrared Resonant Surface-Enhanced Raman Nanoparticles In Vivo. *ACS Nano* **2021,** *15*, 19956–19969.

[2] Yu JH *et al*. Highly Excretable Gold Supraclusters for Translatable *In Vivo* Raman Imaging of Tumors. *ACS Nano* **2023,** *17*, 2554-2567.

I145

APPLICATIONS OF IR AND RAMAN SPECTROSCOPY TO FORENSIC SCIENCE. Marten Seeba[1], Di Yan[1], Antonia Franziska Eckert[1], Felix Fromm[1], and **Peter Krygsman**[2], [1]Bruker Optics Ettlingen, Germany; [2]Bruker td., Milton, ON, Canada.

A long history exists of using vibrational spectroscopy to provide a better understanding of materials collected from sites and taken to the lab and, more recently, where they exist in the environment. In the case of Forensic investigation, particularly InfraRed (IR) and Raman spectroscopy, are well established as important tools for evidence characterization. These spectroscopies are also important to support and inform emergency responders and site management decisions. Bruker's mobile tools for IR and Raman spectroscopy can be deployed to the evidence location. Examples are the BRAVO hand-held Raman system, the MOBILE-IR and ALPHA II IR, plus lesser known but well-developed open path gas analysis instruments, the SIGIS II and OPS gas analysis tools. Spectroscopy in the field can then be supported by careful evidence sample collection and in-depth measurements in the forensic lab using typical FT-IR and Raman systems including microscopes coupled with these spectroscopies. Acceptable sample collection, handling, and preparation for analysis are important for evidence chain of custody and integrity. Reference materials and spectroscopy libraries are important for understanding the evidence. Complicated samples like paint chips are best investigated with microscopes that provide excellent visual documentation and micron scale spectroscopic identification, for example the LUMOS II FT-IR microscope and SENTERRA II Raman Microscope. New developments in these technologies are emerging and more are coming soon. For example, recently developed hybrid IR microscopy combines quantum cascade IR laser sources with typical broadband IR sources. Bruker's Hyperion microscope has both IR sources and now can be added to the tools available to the forensic laboratory.

I146

FORENSIC PROFILING OF 3D PRINTED FIREARMS BY LIBS: PRELIMINARY RESULTS. **Katie Moghadam**[1], Claude Dalpé[2], Nigel Hearns[2], Diane Beauchemin[1], [1]Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON K7L 3N6, Canada; [2]RCMP-GRC National Forensic Laboratory Services, Ottawa, ON K1A 0R2, Canada. (k.moghadam@queensu.ca).

I147

CHARACTERIZATION OF ARSENIC METABOLIC PROFILES USING SIMULTANEOUS ELEMENTAL AND MOLECULAR MASS SPECTROMETRY (HPLC-ICPMS/ESIMS).

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Inorganic arsenic (iAs) is one of the highest priority contaminants. Its elevated concentrations are estimated to affect more than 90 million people worldwide. Simultaneous exposure to iAs and complex organic arsenicals (oAs) may alter arsenic metabolic profiles and, therefore, complicate interpretation of biomonitoring data. To estimate exposure magnitude and metabolic efficiency of iAs, most studies focus on measurement of five arsenic species in urine: arsenite (iAs^{III}), arsenate (iAs^{V}), monomethylarsonic (MMA), dimethylarsinic (DMA) acids, and arsenobetaine (AsB). We first analyzed iAs^{III}, iAs^{V}, DMA, MMA and AsB in 1873 urine samples, provided by the volunteers of Health Effects of Arsenic Longitudinal Study in Araihazar (Bangladesh), using anion exchange high performance liquid chromatography coupled to inductively coupled plasma mass spectrometry (HPLC-ICPMS). Arsenic species had high detection rates (≥ 98%) over broad range of total arsenic concentrations (0.9 to 2633.6 μg/L), except for iAs^{III} which was detected in 71% of the samples. Unknown arsenic peaks were detected in 40.1% of the samples. Further simultaneous elemental and molecular analysis (HPLC-ICPMS/ESIMS) was applied to improve interpretation accuracy of complex metabolic profiles. HPLC-ICPMS/ESIMS method was successfully developed for eleven arsenic species, achieving low detection limits in both ICPMS and ESIMS, and applied for urine samples characterization.

[1] Agency for Toxic Substances and Disease Registry (ATSDR)
https://www.atsdr.cdc.gov/spl/index.html (April 2024)
[2] J. Podgorski, M. Berg, *Science* 368 (2020) 845–850.
[3] T. Davydiuk, J. Tao, X. Lu, X. C. Le, *Environ. Health* 1 (2023) 236–248.

I148

DEVELOPMENT OF LIQUID-BASED AMBIENT ATMOSPHERIC-PRESSURE GLOW DISCHARGES FOR ATOMIC EMISSION SPECTROMETRY,

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A new generation of liquid-based glow discharge plasmas are being developed for atomic spectrometry. The solution-cathode glow discharge (SCGD) is a simple, low power (80W), portable plasma sustained in ambient atmosphere directly upon a sample solution that is being developed for atomic emission spectrometry (AES). The sample solution is directly sampled by the SCGD plasma, with analyte entering the plasma directly to be excited. For many elements, the SCGD offers limits of detection competitive with established techniques like Inductively Coupled Plasma Atomic Emission Spectrometry (ICP-AES). The utility of these liquid-based glow discharge systems for analytical applications will be discussed.

I149

CHALLENGES ON SAMPLE PREPARATION PROCEDURES DUE TO MINIATURIZATION OF INSTRUMENTATION.

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To reap the full benefits of ongoing miniaturization and other advancements in sample analysis instruments, the need for sample prep to keep pace and deliver the requisite reduction in sample size, reagent usage, improved safety, and cost economics have become of paramount importance. Without this balance in sample analysis and sample prep, the overall benefits to analytical labs remain less than optimal. One effective solution to the sample prep challenge lies in enhanced automation in sample prep. Vulcan automated workstation for sample prep delivers accurate yet small quantities of reagents consistently to a large number of small samples in a HEPA filtered, contamination-free environment. The end result delivers better prepared samples ready for modern day spectroscopic analysis.

I150

IDENTIFYING BLOOD PLASMA BIOMARKERS OF ALZHEIMER'S DISEASE THROUGH LASER SPECTRAL ELEMENTAL SIGNATURES AND PROTEOMIC PROFILES.

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disease is a phenomenon that disrupts the normal functioning of components in the body, such as cells, organs, bodily systems like the respiratory and nervous systems, and even mental subsystems, like those dedicated to memory. Liquid biopsy approaches, particularly those involving plasma biomarkers, have the potential to offer noninvasive means of early detection and disease monitoring and have received significant attention in recent years. Alzheimer's disease primarily affects the brain, leading to the progressive loss of cognitive function, including memory, reasoning, and the ability to carry out daily activities. We will report on a series of two studies comparing blood samples from healthy donors and Alzheimer's patients. The first explored how blood metal levels can serve as indicators of disease presence through the use of Laser-Induced Breakdown Spectroscopy (LIBS) and Inductively Coupled Plasma Mass Spectrometry (ICP-MS). Essential metals such as Na, K, Ca, and Mg play a crucial role in maintaining health, and their imbalances can signal disease. In the second study, we analyzed the proteomic profiles of the plasma samples investigated using LIBS and ICP-MS. Using machine learning on LIBS, ICP-MS and proteomics data, we identified significant features that differentiate the healthy samples from the diseased samples ones. Our findings highlight the potential of elemental and proteomic profiles in distinguishing between healthy individuals and those with Alzheimer's diagnosis and provides a step in the potential of laser-based liquid biopsy approaches for disease diagnosis.

I151

STRATEGIES FOR IMPROVING THE DETECTION LIMITS OF SELENIUM NANOPARTICLES BY SINGLE PARTICLE ICP-MS ANALYSIS. **Ruth Merrifield**, PerkinElmer, Woodbridge, ON, Canada.

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LIPIDOMICS ODYSSEY: CURRENT STATUS AND FUTURE HORIZONS. Lise Cougnaud, Reza Maulana, Ana Carolina Dos Santos, Elissa Mariani, Oluwatosin Kuteyi, **Dajana Vuckovic**, Concordia University, 7141 Sherbrooke Street West, Montréal, QC, 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.

I153

ON-LINE LEACHING BIO-ACCESSIBILITY STUDIES OF CANOLA MEAL USING INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Yangyang Wang**, Qiqi Zhang and Diane Beauchemin, Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (15yw103@queensu.ca)

This study investigates the bio-accessibility of potentially toxic elements (Cd and Pb) in canola meal using the continuous online leaching method (COLM) combined with inductively coupled plasma mass spectrometry (ICPMS). Given the sustainability and nutritional benefits of plant-based proteins, canola meal, a high-yield by-product of canola oil production, presents as a potentially promising alternative protein source. However, before it could serve as a food source for human, its potentially toxic element levels and health risks need to be evaluated. This research aims to evaluate the COLM's effectiveness in quantifying these elements' bio-accessible fractions, validate the method's accuracy and precision, and assess the potential health risks of consuming canola meal. Artificial saliva, gastric juice and intestinal juice to simulate human digestion were injected into a flash column packed with 0.1 g of canola meal certified reference material, the effluent flowing into ICPMS. The residue was analyzed using a total digestion method. The results indicate that the leaching profiles of canola meal are not consistent from day to day. Despite these variations, the overall Cd content aligns with the certified value. The overall Pb content was however higher than the certified value. The contamination was likely from the heavy metal content in H_2O_2 used for digestion. The correlation of leaching profiles of Pb isotopes as well as Pb and Cd isotopes indicates a single source of Pb and multiple sources of Cd. The study concludes that the bio-accessibility of Cd in canola meal ranges from 57% to 92% and consuming up to 4.5 kg of canola meal per week would be within safe limits regarding Cd exposure, though further assessment of other toxic elements needs to be done. Future work includes incorporating higher purity H_2O_2, improving the method's precision and repeatability, and incorporating a reaction gas for Cr and As measurement.

I154

RADON DEATH CLOCK: A NOVEL METHOD FOR ASSESSING THE POSTMORTEM INTERVAL WITH RADON. **Behnam Ashrafkhani**[1], Armin Tabesh[1], Fredrik Tamsen[2], Aaron Goodarzi[1], Martin Tondel[3,4], Robert Ian Thompson[1] and Michael Wieser[1], [1]Department of Physics and Astronomy, University of Calgary, Canada; [2]Department of Surgical Sciences, Forensic Medicine, Uppsala Universitet, Sweden; [3]Occupational and Environmental Medicine, Department of Medical Sciences, Uppsala University, Sweden; [4]Occupational and Environmental Medicine, Uppsala University Hospital, Uppsala, Sweden. (behnam.ashrafkhan1@ucalgary.ca)

The determination of the elapsed time since the death of an individual is a challenging problem in forensic science and largely based on biological and biochemical indicators that often yield uncertain results. The goal of this study is to develop a method for post-mortem interval investigation that is not affected by environmental processes. This method is dependent on the decay of radioactive nuclides that accumulate in tissues in the body. In this context, the quantification of long-lived radioactive 222Rn decay products including 210Pb, 210Pb, and 210Bi is employed. Accurate measurement of the relative amounts of selected isotopes enables the determination of the elapsed time since death of the individual. The use of isotope abundance ratios has the advantage that knowledge of the absolute amounts of radon is unnecessary. In this talk, I will present the method and model data to demonstrate how this approach could provide the time of death of an individual with second precision over the period of two weeks. Additionally, variable exposure to radon during life reduces the precision by few hours.