Abstract Booklet

for

The 68th International Conference on Analytical Sciences and Spectroscopy

(ICASS 2026)

Halifax, Nova Scotia

June 17- 19

Author index *click abstract number to hyperlink to abstract within this booklet):*

Author index (*click abstract number to hyperlink to abstract within this booklet*):

Name	Abstract_No.
Sophie Haverstock	T930612
Raymond He	T830114
Kevin Hewitt	T830215
Alison Holliday	P750128
Zeinab Hosseinidoust	T830311
Peter Hwang	T930711
Anna Ignaszak	T730511, T830211
Zhehan Jiang	T82018
Karl Jobst	T82016
Zahra Kanaan	P750120
Voula Kanelis	T930714
Coumba Kanoute	P750124
Lewis Kay	T830711
Matt Kinsella	T840216
Iris Koch	T730415, T81082, T82096
Oleg Krokhin	T92015
Sandeep Kumar	T730414
Caroline Kupczyk	P750938
Sabine Kuss	T740516
Mary Chris Lagumen	T91093
Elaine Lamoureux	T740416
Mathieu Lavallée-Adam	T930111
Chris Le	T92085
Kelly LeBlanc	T81042
Ian Lee	T82056
Tyra Lewis	T72007, T81051
Huiyan Li	T730114
Xing-Fang Li	T730115
Huiyan Li	T741016
Paul Li	T930114
Dhesmon Lima	T92058
Chang Liu	T72005

Name	Abstract_No.
Bob Lockerman	T730411
Kassandra Lok	P750125
Kara Loudon	T71004
Xiufen Lu	P750947
Adam Lynch	P750121
Mengzhen Lyu	T730514
Margaret MacConnachie	T830315
Ella MacPhee	P750642
Sara Mahshid	T82025
Sahar Mahshid	T840218
Bugden Makayla	P750643
Tyler Mallett	T840716
Vaughn Mangal	T82098, T831013
Francesca Marassi	T940718
Sanela Martic	T91031, T930512
Janine Mauzeroll	T81053
Pearse McCarron	T91091
Elizabeth Meiering	T840717
Vicki Meli	T830614
Zach Miller	P750142
Elizabeth Mudge	T740417
Thao Ngyuyen-Tran	T930112
Jessica Ni	P750940
Oluwasayo Oganjinmi	T81045
Richard Oleschuk	T840116
Enea Pagliano	T82085
Adrian Pang	T82095
Patrick Parsons	T81081
Charlotte Polo	P750734
Alexandre Prefontaine	P750122
Darrian Prendergast	T830314
Scott Prosser	T91071

Author index (*click abstract number to hyperlink to abstract within this booklet)*:

T930612

A MULTIPLEXED PLASMONICALLY ENHANCED MICROFLUIDIC DEVICE FOR BACTERIAL DIAGNOSTICS. **Tamer AbdElFatah***; Mahsa Jalali; Carolina del Real Mata; Imman I. Hosseini; Sripadh Guptha Yedire; Geoffrey A. McKay; Rachel Corsini; Roozbeh Siavash Moakhar; Hamed Shieh; Grace Reszetnik; Seyed Vahid Hamidi; Cedric P. Yansouni; Dao Nguyen; Sara Mahshid. McGill University, 3575 Av. du Parc, Montréal QC H2X 3P9, Canada. (tamer.abdelfatah@mail.mcgill.ca).

Nanostructured materials offer unique opportunities for advancing sensing platforms in pathogen diagnostics by enabling enhanced optical responses and accelerated reaction kinetics. By leveraging plasmonic phenomena, such systems can significantly reduce the conventional 48–72 hour diagnostic timeline while supporting accurate pathogen identification and antimicrobial resistance (AMR) profiling. Here, we present a plasmonically enhanced microfluidic device leveraging plasmonic catalysis and structural colorimetry to accelerate both colorimetric molecular identification and phenotypic AMR screening assays. The device integrates loop-mediated isothermal amplification (LAMP) for rapid nucleic acid detection and broth microdilution (BMD) for susceptibility testing within a unified microfluidic architecture. Plasmonic nanostructures enhance local electromagnetic fields, promoting reaction kinetics and enabling direct optical readout through colorimetric shifts. The on-chip LAMP assays target common pathogenic bacteria, including Escherichia coli, Enterococcus spp., Pseudomonas aeruginosa, Staphylococcus aureus, Streptococcus agalactiae, and Streptococcus pneumoniae. Further, the on-chip BMD assay was evaluated against a panel of 12 antibiotics using both Gram-positive and Gram-negative strains. The system achieved 36 minutes turnaround time, 100% identification concordance with the standard MALDI-TOF assay, and 100% essential agreement in AMR profiling relative to conventional BMD assays. Overall, this work establishes a nanostructure-enabled diagnostic sensing system that combines speed, accuracy, and scalability while maintaining gold-standard performance.

T830114

IMPACT OF HILIC STATIONARY PHASE CHEMISTRY ON THE SELECTIVITY AND ELUTION ORDER OF NEUROPATHOLOGICAL GLYCOSPHINGOLIPIDS AND STERYL GLYCOSIDES. **Irina Alecu***[1]; Thao Nguyen-Tran [2]; Steffany A.L. Bennett [3]. Neurolipidomics Lab, India Taylor Lipidomic Research Platform, and Department of Chemistry and Biomolecular Sciences[1]. Ottawa Institute of Systems Biology, Department of Biochemistry, Microbiology and Immunology[2]. University of Ottawa, Ottawa, ON, Canada [3] (ialecu@uottawa.ca).

Analysis and quantification of isomeric lipid species with distinct biological functions necessitates high-resolution chromatographic separation prior to electrospray ionization-tandem mass spectrometry (ESI-MS/MS). In the context of Parkinson's disease (PD), the differentiation and accurate quantification of isomeric hexosylceramides (HexCer) and hexosylcholesterols (HexChol) is critical as a readout for PD disease severity and success of therapeutic interventions. We evaluated the performance of two Hydrophilic Interaction Liquid Chromatography (HILIC) stationary

phases coupled to ESI-MS/MS – unbonded silica and zwitterionic HILIC (HILIC-Z) – for the separation of these challenging isomer pairs. Our results demonstrated that stationary phase selection significantly alters both selectivity and the elution order of HexCer and HexChol isomers. While the HILIC-Z column achieved baseline separation of all HexCer species, it did not adequately resolve the HexChol isomers. The silica column was able to successfully resolve both HexCer and HexChol isomers. Interestingly, while on HILIC-Z, glucosyl-species showed stronger retention, on silica the galactosyl-species eluted second. We also observed that GlcChol and GalChol exhibited disparate electrospray ionization efficiencies. To mitigate potential quantitative bias, we utilized individual standard curves for absolute quantification of each species. This optimized HILIC-ESI-MS/MS framework enables us to separate and accurately quantify these critical isomers to assess differences with regards to age, sex, and PD genotype, offering deeper insights into PD pathomechanism, as well as allowing us to monitor therapeutic efficacy.

T830215

DUAL-FUNCTION AU–MXENE MICRONEEDLES ENABLE DEEP DRUG DELIVERY AND IN SITU LACTATE MONITORING FOR CHRONIC WOUND REPAIR. **Majed Amini***[1,2]; Dragos F. Mantaila [1,2]; Milena Lima [2,3]; Babak Anasori [5]; Hamed Shahsavan[2,4]; Emmanuel Ho [2,3]; Mahla Poudineh[1,2]. [1] Department of Electrical and Computer Engineering, University of Waterloo, Waterloo, ON, Canada; [2] Waterloo Institute for Nanotechnology, University of Waterloo, Waterloo, ON, Canada; [3] School of Pharmacy, Faculty of Science, University of Waterloo, Kitchener, ON, Canada; [4] Department of Chemical Engineering, University of Waterloo, N2L 3G1 Waterloo, Ontario, Canada; [5] School of Mechanical Engineering, Purdue University, West Lafayette, IN, USA (majed.amini@uwaterloo.ca).

Chronic wounds burdened by deep-seated bacterial infections demand simultaneous physiological monitoring and active therapeutic intervention. However, conventional transdermal patches rely on passive diffusion, fundamentally limiting drug penetration depth and real-time diagnostic feedback. Here, we report an integrated, near-infrared responsive microneedle platform that combines in situ lactate biosensing with hydrogen-propelled deep drug delivery for chronic wound repair. The dual module system comprises a swellable sensing array incorporating an aptamer MXene complex to detect infection biomarkers, alongside an anisotropic delivery array. The delivery microneedles feature a fully crosslinked methacrylated hyaluronic acid base doped with a catalytic Au MXene heterostructure, physically integrated with a half crosslinked, ciprofloxacin-loaded tip. Under near infrared irradiation, rapid interfacial charge transfer within the Au MXene matrix drives localized gas-related behavior. This externally triggered reaction generates a measurable hydrogen signal and facilitates enhanced local transport, actively propelling the antimicrobial payload up to 1000 μm into the tissue. Evaluated across in vitro and in vivo featuring a mixed S. aureus and P. aeruginosa infection, this active propulsion strategy demonstrated superior antibacterial efficacy and significantly accelerated wound closure. Ultimately, this design establishes a robust route for

externally triggered wound microneedles, providing a highly capable platform for active transdermal therapy and continuous monitoring.

P750128

DETECTING AND QUANTIFYING TOXIC DEOXYNIVALENOL DERIVATIVES IN CEREAL GRAINS USING TANDEM MASS SPECTROEMTRY. **Radwa Asar***[1]; Maria Alejandra Oviedo-Ludena [2]; Lipu Wang [2]; Randy Kutcher [2]; and Anas El-Aneed [1]. [1] College of Pharmacy and Nutrition, University of Saskatchewan, Saskatoon, SK, S7N 5E5, Canada; [2] Department of Plant Sciences, University of Saskatchewan, Saskatoon, SK S7N 5A8, Canada (rra016@mail.usask.ca).

Fusarium head blight (FHB) is a fungal disease that affects cereal crops worldwide. The etiology of the disease is associated with the production of mycotoxins, primarily deoxynivalenol (DON), which contaminate grains, resulting in low crop quality and health risks for consumers. However, plant-modified derivatives, known as “masked mycotoxins” have been identified and these derivatives escape standard analysis and can revert to their toxic parent compounds upon digestion. Our work demonstrates the development of a simple, quick, and sensitive liquid chromatography tandem mass spectrometry (LC-MS/MS) method for the detection and quantification of DON and its masked derivative, deoxynivalenol glucoside (D3G), in Canadian cereal grains. The method was developed using a TSQ Altis® triple quadrupole MS with an electrospray ionization source in negative ion mode. In addition, we tested the utility of a single point calibration approach, demonstrating, for the first time, that accurate results are attainable without the need for convectional quantitative workflow. The method was validated as per SANTE guidelines (EU) on three grains and applied to 116 cultivars, supporting monitoring, plant breeding programmes, food safety, and FHB management strategies.

T830311

SOME RECENT CASE STUDIES IN HERITAGE SCIENCE AT THE CANADIAN CONSERVATION INSTITUTE. **Stephanie Barnes***. Canadian Conservation Institute, 1030 Innes Road, Ottawa, ON K1B 4S7, Canada (stephanie.barness@pch.gc.ca).

This presentation will introduce the work done by the Conservation Science Division of the Canadian Conservation Institute, a small agency within the department of Canadian Heritage that works to study, preserve and protect cultural heritage. Conservation Scientists work at the intersection between science and art to answer questions about art and heritage objects using a broad range of spectroscopy, spectrometry, microscopy, and photographic techniques. Case studies with links to the East Coast (including paintings, textiles and maps) will be presented, with a focus on the multianalytical approach chosen based on the project. The types of results which can have applications in forensic conservation science – the use of science to assist law enforcement and combat art fraud – will also be addressed

T82017

IDENTIFICATION OF SPECIFIC VETERINARY DRUG RESIDUES FOR MORANTEL AND PYRANTEL, APPLICABLE FOR USE IN MCLA SCREENING. **Amir Sedigheh Barzegar***[1,2]; Bryn O. Shurmer [2]; Anas El-Aneed [1,2]; and Randy W. Purves [1]. [1] College of Pharmacy and Nutrition; University of Saskatchewan, Saskatoon SK S7N 5E5, Canada; [2] Centre for Veterinary Drug Residues{2], Canadian Food Inspection Agency, Saskatoon, SK S7N 2R3, Canada. (bmy018@usask.ca).

The Canadian Food Inspection Agency regularly tests animal-derived food products to ensure veterinary drug residues (VDRs) comply with levels established for regulated drugs. The current regulatory method for morantel/pyrantel is effective, however, it involves a laborious, time-consuming procedure and produces a nonspecific VDR that cannot distinguish these two drugs. Our objective was to identify specific metabolites for use in a targeted multi-residue (MCLA) screening method. In vitro incubations with liver S9 fractions were used to generate metabolites. Samples were analyzed using liquid chromatography – high-resolution mass spectrometry (LC–HRMS), and compound discoverer software assisted with metabolite identification. Using mixtures of stable isotope 13CD3-labeled standards and unlabeled standards supported the identification of major morantel/pyrantel metabolites, by showing two peaks 4.0219 m/z apart. Major metabolites across several species were observed resulting from hydroxylation, reduction, and cysteine conjugation bio-transformation reactions. MS/MS and MS3 were used to determine metabolic reaction sites and structures. Major metabolites identified using pseudo-incurred liver tissues were consistent with the in vitro results. Using specific morantel and pyrantel metabolites overcomes the lack of specificity associated with the current regulatory method. This metabolite-based detection workflow is rapid and compatible with MCLA methods, and readily adaptable to other veterinary drugs.

P750729

RECOMBINANT CRIBELLATE SPIDER SILK: LINKING MOLECULAR DESIGN TO MECHANICAL PROPERTIES. **Hina Batool***[1]; Woobeen Shin [1]; Suad Rashid [1]; Jan K. Rainey [1,3]. Department of Biochemistry & Molecular Biology, Dalhousie University, Halifax, NS, B3H 4R2, Canada [1]; Department of Chemistry, Dalhousie University, Halifax, NS, B3H 4R2, Canada [2]; School of Biomedical Engineering, Dalhousie University, Halifax, NS, B3H 4R2, Canada [3]. (hn701981@dal.ca).

Spider silks are remarkable biomaterials combining strength, extensibility, and toughness. Among the various silk types, prey capture silks are particularly important to spiders' ecological success, enabling them to intercept and retain wriggling prey without snapping. While ecribellate spiders' viscid capture silk has been extensively studied, the dry-adhesive cribellar nanofibrils composing cribellate capture threads remain poorly characterized at the molecular level To investigate the structural basis of cribellate silk, a recombinant construct, CrR1312, containing four repeat units

from the cribellate orb-weaver Uloborus diversus was expressed, purified, and spun into fibres. Mechanical characterization confirmed exceptionally high extensibility (~242%) and tensile strength tunable by post-spin stretching (~44 to ~132 MPa). Structural analysis revealed α-helical conformation in solution, transitioning upon fibre formation into increased β-sheet content with enhanced molecular alignment. Solution-state NMR revealed coexisting folded and disordered regions — potentially analogous to ecribellate silks despite lengthy evolutionary divergence, suggesting convergent structural strategies underlying capture silk mechanics. Future work will focus on backbone dynamics and relaxation analysis of cribellate spidroin to analyze the interplay between ordered and disordered domains during fibre assembly.

T91013

DIFFERENTIAL ION MOBILITY SPECTROMETRY FOR SEPARATION OF NATURAL TOXINS. **Daniel G. Beach***. Metrology Research Centre, National Research Council, Halifax, NS (Daniel.Beach@nrc-cnrc.gc.ca).

Differential ion mobility spectrometry separations (DMS or FAIMS), are gas phase ion filters that operates at atmospheric pressure after electrospray ionization before the inlet to a mass spectrometer. They separate ions based on size, shape and charge and can be orthogonal to polarity-based separations in LC and m/z. Because of high chemical background at low m/z, DMS and FAIMS have been used to increase signal-to-noise and improve selectivity in LC-MS/MS analysis of small polar natural toxins. For the putative cyanobacterial neurotoxin β-N-methylamino-L-alanine (BMAA), which has been controversial because of poor analytical selectivity and in complex hydrolyzed environmental and biological samples, improved LOD and complete resolution from interfering isomers was achieved by HILIC–DMS–MS/MS. Recent work has focused on developing less targeted approaches with FIAMS using high resolution mass spectrometry, for comprehensive profiling of cyanobacterial secondary metabolites. Here, FAIMS could be operated as a wide-pass filter with LC to focus precursor-ion selection or used as a primary separation tool without LC. Data acquisition in ESI-FAIMS-HRMS/MS is not limited by chromatographic peak width, and compensation voltage (the main experimental variable) can be scanned at any rate or paused for precursor ion accumulation, allowing for unique approaches to non-target analysis.

T731013

INFRARED-HEATED SAMPLE INTRODUCTION SYSTEM TO ENHANCE TRANSPORT EFFICIENCY FOR YEAST CELL ANALYSIS BY SINGLE CELL INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Diane Beauchemin***; Zichao Zhou, Mirah J. Burgene; John Burgener. Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada (diane.beauchemin@queensu.ca).

The analytical performance of single cell inductively coupled plasma mass spectrometry (scICPMS) for the quantitative analysis of individual cells is strongly constrained by sample transport efficiency (TE). In this work, an infrared (IR)–heated pneumatic sample introduction system based on a modified cyclonic spray chamber, where the aerosol is pre-evaporated without solvent removal prior to entering the plasma, was employed for scICPMS analysis of a Se-enriched Saccharomyces cerevisiae (yeast) certified reference material. Multivariate optimization of IR-heating temperature, nebulizer gas flow rate, sample uptake rate, and sampling position was conducted. At 150 °C and 5 μL min^{-1}, the IR-heated system achieved a cell TE of 47 ± 6%, representing a substantial improvement versus a conventional cyclonic spray chamber (1.1 ± 0.4%) and exceeding that of a commercial single cell introduction system (30 ± 3%). Detection limits of 100–120 ag per cell were achieved for ^{78}Se and ^{82}Se. The measured 65–68 fg Se $cell^{-1}$ is consistent with independent estimates derived from certified total Se concentration and bulk digestion measurements. Cell lysis occurred at IR-heating temperatures above 220 °C. Overall, controlled IR-heated sample introduction significantly enhances transport efficiency and enables reliable Se quantification in cells without requiring independent transport efficiency calibration.

T740418

EVALUATING THE BIOACCESSIBILITY OF TRACE METALS IN A PLANT BASED ALTERNATIVE PROTEIN SOURCE, CANOLA MEAL, USING ONLINE LEACHING METHOD COUPLED TO INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Diane Beauchemin***; Yangyang Wang; Qiqi Zhang. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada. (diane.beauchemin@queensu.ca).

Sustainable plant-based proteins are gaining attention as alternatives to conventional animal based protein sources, driven by growing environmental and food security concerns. In this study, the bioaccessible fractions of trace elements including Ti, V, Cr, Co, Ni, Cu, Zn, Sr, Mo, Cd, Ba, and Pb were measured in canola meal. A continuous online leaching method (COLM) coupled with inductively coupled plasma mass spectrometry was used to simulate human digestion, where artificial saliva, gastric juice, and intestinal fluid were sequentially passed through a mini column of canola meal. Internal standards in the artificial fluids corrected for column-related variability, improving median standard deviations by two-fold with significant improvement for Co, Cu, Cd, and Ba, median limits of detection by seven-fold, and recoveries for Co, Ni, Cu, Zn, Sr, Cd, Ba, Pb. The performance of the method and its bioaccessibility results were compared with those using a batch method. Release dynamics were investigated through cumulative signal profiles and isotopic ratio analysis. Additionally, scenario-based exposure assessments were carried out across different sex and age groups. This study shows that the COLM provides complementary bioaccessibility information to conventional total concentration measurements, offering a more realistic and comprehensive basis for food safety and nutritional assessments.

T81013

PATHWAY STRENGTH: A BIOINFORMATIC ALGORITHM THAT COMPUTES THE BIDIRECTIONAL STRENGTH OF METABOLIC PATHWAYS FROM STEADY STATE LIPIDOMIC. **Steffany A.L. Bennett***[1]; Zach Miller [1]; Miroslava Cuperlovic-Culf [2]; Thao Nguyen-Tran [1]. [1] Neurolipidomics Lab, India Taylor Lipidomic Research Platform, Ottawa Institute of Systems Biology, Department of Chemistry and Biomolecular Sciences and Department of Biochemistry, Microbiology and Immunology, University of Ottawa; [2] Digital Technologies Research Centre, National Research Council of Canada, Canada, Ottawa, ON. (steffanyAnn.Bennett@uottawa.ca).

Lipidomic signatures in biofluids are under assessment as potential prognostic and monitoring biomarkers. The metabolic interpretation of these steady-state signatures is often challenging due to (1) the diversity and complexity of the lipidome, (2) the interconnection of lipid metabolism wherein the level of each lipid molecule is the result of multiple enzymatic reactions, and thus (3) statistical changes (or lack thereof) in lipid abundances is not simply a direct result of a mutation but rather a snapshot of a change of state across the entire metabolic system. We present here a strategy to derive a clinically relevant metabolic index of this change in state from steady-state lipidomics acquired using nanobore reversed-phase liquid chromatography-electrospray ionization-differential mobility spectrometry, tandem mass spectrometry (RPLC-ESI-DMS-MS/MS) followed by information-dependent-acquisition of enhanced product ion scan (IDA-EPI) in different matrices. This index was developed and validated in cell culture treated with enzymatic inhibitors and deployed in assessment of plasma samples from GBA1-Parkinson's patients. We report here our quantification of β-GlcCers and β-GalCers, as well as β-GlcChol and β-GalChol and show that the expression of GBA1-PD variants alters GBA1's transferase activity (a novel gain of GBA1 enzymatic function) in human plasma.

T81091

TWENTY YEARS OF ENVIRONMENTAL MONITORING AT THE CENTRE FOR WATER RESOURCES STUDIES CLEAN WATER LAB – HIGHLIGHTS, REFLECTIONS, AND FUTURE DIRECTIONS. **Jessica L. Bennett***; Graham A. Gagnon. Centre for Water Resources Studies, Department of Civil & Resource Engineering, Dalhousie University (J.Bennett@dal.ca).

Understanding the fate and presence of trace organic compounds in water holds significant importance for both human and environmental health. Here, we reflect on the last twenty years of environmental monitoring and mass spectrometry work at the Centre for Water Resources Studies Clean Water Laboratory. We outline the evolution of our analytical methods across domains and water matrices, and discuss progress, challenges, and technical lessons learned over decades. Key milestones will be highlighted, including development and evolution of a passive sampling approach for cyanotoxin monitoring in recreational and drinking waters, development and validation of two QuEChERS methods for isolation of steroid estrogens from wastewater and waste solids in aquaculture systems, and our recent implementation of a modified EPA 533 method for isolation and

quantitation of PFAS in drinking water and beyond. Finally, we will outline our next steps and future directions, including our planned upgrade to a high-resolution mass spectrometer which will enable suspect screening and retrospective data analysis. This upgrade in analytical capability will enhance our ability to detect and identify emergent contaminants and advance our knowledge in treatment and design across the water sector.

P750646

APTAMER-BASED BIOMARKER DETECTION FOR MUSCLE HEALTH MONITORING. **Jenna Berryman***[1]; Christa L. Brosseau [1]; Rafaela Andrade [2]. [1] Department of Chemistry, Saint Mary's University, Halifax, NS, Canada; [2] Myomar Molecular Inc., Halifax, NS, Canada (Jenna.Berryman@smu.ca).

Sarcopenia, the age-related decline in skeletal muscle mass and function, is associated with increased risks of frailty, metabolic disorders, and mortality. Despite its clinical significance, routine monitoring remains limited by reliance on expensive and inaccessible diagnostic techniques. This work investigates the development of complementary aptamer-based assays for the detection of a urinary biomarker associated with muscle metabolism. A fluorescencent intercalator displacement (FID) assay was used to characterize aptamer–target interactions and quantify the biomarker. In parallel, a competitive lateral flow assay incorporating gold nanoparticle–aptamer conjugates was developed for rapid, visual detection. Analytical performance was evaluated using external calibration, spike-and-recovery experiments, and analysis of urine matrices to assess sensitivity, selectivity, and matrix compatibility. These results demonstrate the feasibility of integrating fluorescence and lateral flow platforms for sensitive and non-invasive detection, highlighting their potential as accessible point-of-care tools for monitoring muscle health.

T82058

ELECTROOXIDATION OF UREA: INVESTIGATING PRODUCTS FORMATION AND STABILITY OF THE CATALYSTS. **Noah Ruscica***; Erwan Bertin. St Francis Xavier University, Department of Chemistry 5009 Chapel Square, Antigonish, NS B2G 2W5 Canada (ebertin@stfx.ca).

Urea is one of the most common waste products that can present a hazard to aquatic life and human health. Its removal via electrochemical oxidation has been proposed over a decade ago on Ni based catalysts.1 The products formed were assumed to be N2 until the work of Li et al2 who demonstrated in 2022 that the major products were actually NO2- and NCO-. Thus, we reinvestigated some of our catalysts (Ni, NixFe100-x and NixCu100-x), aiming to assess the products formed by ion chromatography. Our results also showed that NO2- was the main product observed, with no significant change in selectivity observed over 12h. Investigation by atomic spectroscopy did reveal good catalyst stability, with the dissolution of less than 2% of the catalyst during that period.

T830115

ANALYSIS OF GEOLOGICAL SAMPLES USING A LIQUID MICROJUNCTION SAMPLE INTRODUCTION SYSTEM FOR INDUCTIVELY COUPLED PLASMA MASS SPECTROMETRY. **Alexander W. Bewsh***; Diane Beauchemin. Queen's University,Department of Chemistry, 90 Bader Lane, Kingston, ON, K7L 3N6, Canada. (alex.bewsh@queensu.ca).

The increasing demand for critical minerals, necessitates the development of strategies allowing the quick identification of domestic mineral deposits. Inductively coupled plasma mass spectrometry (ICPMS) remains a key technique for analysis of geological materials due to its high specificity and sensitivity; however, it can require extensive and time-consuming sample preparation if the sample is in solid form. Direct solid analysis techniques such as laser ablation or electrothermal vaporization coupled to ICPMS can be used to circumnavigate most sample preparation steps but are limited by high instrument acquisition costs. This work presents a cost effective liquid microjunction surface sampling probe (LMJ-SSP) coupled with ICPMS for the determination of rare earths, noble metals, and other elements in critical minerals. This probe enables analyte leaching through the formation of a liquid bridge between two coaxial capillaries and a sample surface. Leaching conditions for complex geological matrices were optimized tomaximize sensitivity, and quantitative capabilities of the probe were evaluated. Plasma robustness was also assessed by comparing the levels of oxide and doubly charged interferences to those experienced using conventional flow injection analysis.

T92016

A COMPARISON OF MULTIDIMENSIONAL SEPARATION TECHNIQUES FOR THE IDENTIFICATION AND QUANTIFICATION OF MICRO-/NANOPLASTICS BY PYROLYSIS GC-MS. **Justine R. Bissonnette***; Emmanuel C. Tolefe; Nikita E. Harvey; Lindsay S. Cahill; Karl J. Jobst. Department of Chemistry, Memorial University of Newfoundland, 45 Arctic Ave., St. John's, Newfoundland and Labrador, Canada (jbissonnette@mun.ca).

Pyrolysis - gas chromatography mass spectrometry (Py-GCMS) is a promising technique for quantitative analysis of micro-/nanoplastics (MNPs); however, matrix effects from lipid-rich biological samples can compromise analytical accuracy. Drift time and collision cross section (CCS) calculations obtained from pyrolysis - gas chromatography × cyclic ion mobility mass spectrometry (Py-GCxcIMS) can be used to distinguish MNP analyte ions from matrix interferences [1]. Two-dimensional gas chromatography (GCxGC-MS) offers an alternative approach that may reduce matrix effects, though it remains underexplored for MNP analysis. In this study, Py-GCxcIMS, Py-GCxGC-MS, and Py-GCxGCxcIMS were compared for the quantification of MNPs in base-digested human blood. Multiplicative matrix effects were assessed by comparing instrument responses (area counts) from MNP standards prepared with and without matrix. Base-digested lipid standards, including fatty acids (arachidonic acid, oleic acid, palmitic acid, and lignoceric acid) and a phospholipid (phosphatidylcholine), were used to evaluate each method's ability to separate lipid-

derived interferences from genuine MNPs. Overall, this work aims to reproduce previously observed interferences [1] and identify the most effective method for differentiating them from MNP detections.

T740116

SCALABLE AND COST-EFFECTIVE ABSOLUTE QUANTIFICATION OF THE HUMAN PROTEOME USING SYSQUAN. **Christoph H. Borchers***[1,2,3,4]; Timon Geib [1], Elodie Logerot [1]; Peter Kubiniok [5]; Victor Spicer [6]; Stoyan Stoychev [7]; Robert Popp [8]; René P. Zahedi [6,9,10,11]; Dorte B. Bekker-Jensen [7]; and Nicolai Bache [7]. [1] Segal Cancer Proteomics Centre, Jewish General Hospital, Montreal, QC, Canada ; [2] Gerald Bronfman Department of Oncology, Jewish General Hospital, Montreal, QC, Canada; [3] Division of Experimental Medicine, McGill University Montreal, QC, Canada; [4] Department of Pathology, McGill University, Montreal, QC, Canada; [5] Quantivum Inc, Montreal, QC, Canada; [6] Manitoba Centre for Proteomics and Systems Biology, Winnipeg, MB, Canada; [7] Evosep Biosystems, Odense, Denmark; [8] MRM Proteomics, Inc, Montreal, QC, Canada; [9] Department of Internal Medicine, University of Manitoba, Winnipeg, MB, Canada; [10] Department of Biochemistry and Medical Genetics, University of Manitoba, Winnipeg, MB, Canada; [11] Paul Albrechtsen Research Institute, CancerCare Manitoba, Winnipeg, MB, Canada. (christoph.borchers@mcgill.ca).

Quantitative proteomics is often limited by matrix and batch effects, complex workflows, and long chromatographic methods, which hinder detection of subtle biological changes and reduce reproducibility across laboratories. In addition, the high cost and limited availability of stable isotope-labeled (SIL) standards restrict widespread implementation of absolute quantification. SysQuan overcomes these limitations by using SIL mice as a universal internal standard, enabling scalable and cost-efficient absolute quantification across tissues. C57BL/6 mice were metabolically labeled with 13C-lysine to generate SIL reference material. Human and SIL mouse plasma and tissues were mixed 1:1, processed via S-Trap digestion, and analyzed using both targeted dynamic MRM on an Agilent 6495D Triple Quadrupole coupled to an Evosep One LC system, and untargeted workflows on timsTOF HT mass spectrometer and Orbitrap Exploris 480 platforms. Across plasma and tissues, thousands of proteins and tens of thousands of SIL peptide pairs were quantified. More than 2,500 MRM assays were developed per tissue, enabling high-throughput targeted analysis. Reverse quantification of SIL standards allows calibration-free workflows, while validated concentrations in SIL plasma support single-run absolute quantification. Using streamlined sample preparation and one-hour LC-MS runs, SysQuan enables robust quantification of hundreds of plasma proteins with high reproducibility.This approach substantially reduces cost and complexity, making large-scale absolute proteome quantification broadly accessible.

T730113

SIMPLE ON THE SURFACE: SINGLE-STEP FABRICATION OF MOLECULARLY IMPRINTED POLYMERS THIN-FILMS FOR SAMPLING AND DIRECT INTERFACE TO MASS SPECTROMETRY. **Christina Bottaro***; Reza Akhoondi; Ali Azizi; Evan Langille; Temitope Nwachukwu; Omid Qanati, Sophia Parent; Fereshteh Shahhoseini. Memorial University of Newfoundland, Department of Chemistry, 45 Arctic Avenue, St. John's, NL A1C 5S7, Canada (cbottaro@mun.ca).

Porous polymeric coatings can be made using simple one or two-step fabrication methods with high atom economy to create devices for thin-film microextraction (TFME). A countless variety of functional monomers are available for the creation of these porous organic covalent networks that can be tailored for selectivity, porosity, surface area, and sample compatibility. The addition of molecular imprinting, in which a template molecule provides a scaffold (self-assembly before polymerization) for monomers, favourably orients functional groups at the binding sites to increase binding affinity for analytes. Polymer porosity can also be tuned to balance the surface area needed for high extraction efficiency (microporous) against desirable mass-transfer dynamics (macroporous), which is of particular concern during direct MS interrogation where quick desorption is crucial. In this talk, challenges associated with optimization of polymer performance, methods to understand selectivity, and the use of design of experiment to refine materials will be highlighted. Data from UHPLC-MS/MS, direct introduction to MS (blade-spray), and a hand-held mass spectrometer (MX908) will be presented to highlight the adaptability of the coated blade format, along with the utility of a coated mesh device for ultra-trace pesticide analysis.

T930614

QUANTITATIVE ISOTOPE-RESOLVED SERS FOR RAPID ANTIBIOTIC SUSCEPTIBILITY. **Ryma Boudries***; Malama Chisanga. Dalhousie University, Department of Chemistry, 6243 Alumni Crescent, Halifax, NS B3H 4R2, Canada (r.boudries@dal.ca).

Rapid antibiotic susceptibility testing (AST) requires analytical methods capable of detecting and quantifying early metabolic responses to antibiotic exposure. Here, we present a surface-enhanced Raman scattering (SERS)-based analytical approach for phenotypic AST using 15N isotopic labeling to directly measure bacterial metabolic activity. The method relies on the incorporation of 15N-enriched nitrogen sources into newly grown bacteria, producing measurable spectral shifts and intensity variations in SERS signatures. Bacterial populations are exposed to antibiotics in presence of 15N-labeled nutrients, enabling quantitative assessment of metabolic activity through isotope-dependent spectral features. Changes in vibrational band positions and relative peak intensities are used to detect and quantify isotope incorporation, providing a direct metric of biosynthetic activity. The high sensitivity and molecular specificity of SERS enable detection of subtle biochemical changes at low bacterial concentrations and short incubation times. This approach provides quantitative insight into nitrogen assimilation and biomolecular synthesis pathways, enabling early measurement of antibiotic-induced metabolic suppression. Preliminary measurements

demonstrate that isotope-dependent spectral markers can be detected and quantified reproducibly, allowing classification of antibiotic susceptibility based on metabolic response. The proposed method establishes a quantitative analytical framework for isotope-resolved SERS measurements and highlights the potential of 15N labeling for rapid phenotypic AST and metabolic profiling.

T82057

PLASMONIC MATERIALS IN ELECTROCHEMISTRY AND PHOTOCATALYSIS. **Alexandre G. Brolo***. University of Victoria, Department of Chemistry, Victoria, BC, Canada (agbrolo@uvic.ca).

The quest for new types and approaches for photocatalysis is a very active field, since highly efficient synthesis should play a pivotal role in a sustainable future. Recently, a large amount of attention has been dedicated to the exploration of electrochemical and photocatalysts based on plasmonic materials. In this work, we studied a self-assembled monolayer of 4-mercaptobenzenenitrile (4-MBN), which is a relatively stable molecule

widely used as a label in surface-enhanced Raman experiments. The 4-MBN monolayer was deposited on a nanostructured Au surface. Far-field spectra at different laser powers confirmed the resilience of this monolayer, with carbonization being recorded at laser power densities higher than 127.3 MW/cm2. In contrast, experiments in the near field showed not only the onset of the decomposition at significantly lower power densities of 4

MW/cm2, but also that the decomposition products did not show the presence of carbonization. The spectra obtained using near field excitation suggest selective chemical functionalization driven by the near field conditions. These results were interpreted by the near field activation of dark plasmon modes that provide a distinct reaction pathway for the chemical process. Electrochemical experiments exploring the reduction of carbon dioxide will also be presented.

T830612

ADVANCING ELETROCHEMICAL SERS USING SCREEN-PRINTED ELECTRODES. **Christa L. Brosseau***; Claire Cullinan; Mary Stackaruk. Department of Chemistry, Saint Mary's University, Halifax, NS, Canada, B3H 3C3 (christa.brosseau@smu.ca).

Electrochemical surface-enhanced Raman spectroscopy (EC-SERS) has been in existence since the first SERS observation 50 years ago this year. Recently, there has been a significant increase in the use of EC-SERS for scientific studies, largely due to the availability of portable instrumentation at reduced cost. Over the past 15 years, our research group has explored screen printed electrodes (SPEs) as a platform for routine spectroelectrochemical investigations, which combine SERS and electrochemistry. In this talk, I will outline the various ways in which we fabricate screen-printed electrodes for use in EC-SERS measurements and will discuss applications of the technique, including biosensor development and thin-film investigations.

P750730

COMBINED USE OF 1H RELAXATION AND J COUPLINGS TO DETERMINE PROTEIN SIDE CHAIN DIHEDRAL ANGLES. **Shaista Goel***; Jingyang Bu; David Case; Peter Hwang. Department of Biochemistry, 3-08 Medical Sciences Building (jbu3@ualberta.ca).

The Karplus equation describes the relationship between three-bond NMR J couplings and the dihedral angle θ defined by the three bonds: □□ = □□0 + □□1 cos(□□) + □□2cos (2□□) C0, C1, and C2 depend on the atoms involved, derived empirically or from quantum mechanical calculations. We performed NMR quantitative J coupling experiments, HNHB, HN(CO)HB, and H-TOCSY CHSQC, to measure side chain χ1-dihedral angle-dependent J couplings between HB2/3 protons and backbone N, CO, and HA atoms, respectively, in the WW domain of human Pin1 protein. When the atoms are in a trans (180º) configuration, there is large J coupling between them, and when they are gauche (60º), it is small. When a side chain is highly mobile, the J couplings are averaged. J couplings can be fit to a single side chain χ1-dihedral angle for a rigid residue or to a mixture of the three major rotamers for a mobile residue. It is often impossible to determine the correct model based on J couplings alone, so we used 1H-NMR relaxation rates to distinguish rigid from mobile residues. The most commonly used Karplus coefficients yielded spurious results for the most rigid residues in Pin1, so we used density functional theory to calculate new coefficients for the NMR community.

T730512

LEVERAGING MASS TRANSPORT IN SCANNING ELECTROCHEMICAL CELL MICROSCOPY FOR QUANTITATIVE ELECTROANALYSIS. **Joshua C. Byers***; Samaneh Salek. Département de Chimie, Université du Québec à Montréal Montréal, Québec, Canada (byers.joshua@uqam.ca).

Scanning Electrochemical Cell Microscopy (SECCM) is a powerful technique for probing electrochemical processes at the micro- and nanoscale, enabling high-spatial-resolution electrochemical measurements. By using a pipet probe to form a confined meniscus electrochemical cell, SECCM has been widely applied to investigate functional electrode materials including individual particles. Recently, we have begun to explore the role that mass transport can play during SECCM measurements for the oxygen reduction reaction. In this work, recent results exploring two different systems will be presented to highlight the effects of mass transport during SECCM measurements. In the first example, we investigate the influence of pipet diameter on mass transport rates in the room temperature ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate. The experimental results are compared with finite element simulations and analytical expressions to determine the diffusion coefficient and heterogeneous rate constant for ferrocene at a glassy carbon substrate. In the second example, we employ SECCM to study the kinetics of the oxygen reduction reaction on individual platinum nanoparticles in acidic media, which is a benchmark catalyst for this

reaction. By leveraging SECCM's high spatial resolution, we correlate electrochemical activity with individual particle size to enable quantitative analysis of these materials

T92056

MEASURING ELECTRON-TRANSFER REACTION KINETICS IN SINGLE ELECTROCHEMILUMINESCENCE EVENTS AT AN ULTRAMICROELECTRODE FOR THE RU(BPY)/TRI-N-PROPYLAMINE COREACTANT SYSTEM. **Zhenzhong Cai***; Tianyu Wei; Zhifeng Ding. Western University, Department of Chemistry, 1151 Richmond Steet, London, ON N6A5B7, Canada (zcai66@uwo.ca).

Electrochemiluminescence (ECL) provides a powerful approach for probing fast electron-transfer reactions through time-resolved photon emission. Here we demonstrate a time-resolved ECL strategy that enables direct determination of charge-transfer rate constants in the benchmark Ru(bpy)32+ /tri-n-propylamine system. By combining ultramicroelectrode potential pulsing with nanosecond-resolved photon counting, the time evolution of ECL emission was measured in the sub-millisecond regime where electron-transfer kinetics control the signal. Finite-element simulations were used to analyze the coupled diffusion and reaction processes and extract rate constants from the experimental data. This approach enables quantitative determination of key homogeneous charge-transfer steps responsible for excited-state generation and provides mechanistic insight into the reaction network underlying coreactant ECL. The methodology establishes a general electrochemical framework for resolving fast kinetics in ECL systems and can be extended to other luminophores and coreactants.

T81054

ELECHEMICAL AND IN SITU FTIR SPECTROSCOPIC PROBING OF NANOSTRUCTURED CATALYSTS FOR SUSTAINABLE ENERGY APPLICATIONS. **Aicheng Chen***. University of Guelph, Department of Chemistry, 50 Stone Road East, Guelph, ON N1G 2W1, Canada (aicheng@uoguelph.ca).

With rapidly escalating environmental concerns and the accelerated depletion of fossil fuel resources, there is an urgent demand for the development of advanced technologies for sustainable energy production. Nanostructured materials with high surface areas have attracted significant interest owing to their unique physicochemical properties and their wide-ranging applications in electrocatalysis, photocatalysis, energy conversion, and energy storage. In recent years, our research team has designed and systematically investigated a diverse range of functional nanomaterials. In this talk, we present the design and synthesis of advanced cobalt-, bismuth-, ruthenium-, and graphene-based nanomaterials and nanocomposites. These materials were comprehensively characterized using a suite of surface and structural techniques. The electrochemical properties of these nanomaterials, as well as their promising applications in

hydrogen production and carbon dioxide reduction, are highlighted. The products generated from the CO2 electrochemical reduction were identified by gas chromatography and nuclear magnetic resonance (NMR) spectroscopy. The kinetics of the CO2 reduction reaction at nanostructured catalysts were further studied using in situ electrochemical Fourier transform infrared (FTIR) spectroscopy. The critical roles of nanostructured surfaces in water splitting and the electrochemical reduction of CO2 are discussed.

T930515

USING ELECTROCHEMISTRY TO DETECT ESCHERICHIA COLI AND ANTIBIOTIC-RESISTANT BACTERIA BY MONITORING BIOMOLECULES. **Rebecca X. Y. Chen***; Zhe She; R. Stephen Brown. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON K7L 3N6, Canada (21rxyc@queensu.ca).

A contaminant of emerging concern with significant impact on the environment and in clinical settings is antibiotic-resistant bacteria (ARB). The Council of Canadian Academies reported that ARB caused an estimated 14,000 deaths and antimicrobial resistance related expenses cost the Canadian healthcare system $1.4 billion in 2018. Current methods for detecting ARB rely on culturing in lab facilities, use analytical instrumentation with trained personnel, and can take 48 hours or more to obtain results. These methods cannot be used for rapid and routine testing or real-time on-site monitoring of ARB, especially in remote areas. We must be able to detect and monitor ARB to understand its trends of release, spread, exposure, and infection to inform effective treatment and policy. Portable biosensors, such as the blood glucose meter, home pregnancy test, and COVID 19 rapid tests, show how accessible testing enables people to rapidly screen their health and decide whether to seek further medical care. Biosensors can also be used in other settings and applications including monitoring environmental health. Development of a portable, easy-to-use biosensor for ARB eliminates the need for expensive analytical instruments and trained personnel. This research combines electrochemical and microbiological detection to address the demand for low-cost, portable, rapid, sensitive, and specific in-situ detection and identification of ARB. Electrochemical biosensorsfor bacteria and ARB detection can be designed for direct detection, such as by antibody binding, or indirect detection by detecting indicator biomolecules specific to the microbes as is effectively demonstrated in this work. The versatility of biosensor designs and miniaturization capabilities of electrochemical systems presents an opportunity to develop a portable multiplexed electrochemical biosensor for multiple bacterial and ARB analytes.

P750328

NON-DESTRUCTIVE MULTI-ELEMENT CHARACTERIZATION OF POLYMER MATERIALS FOR FORENSIC APPLICATIONS BY A LIQUID MICROJUNCTION SMAPLING INTO INDUCTIVELY COUPLED

PLASMA MASS SPECTROMETRY. **Jordan Chiabai*;** Diane Beauchemin. Queen's University, Department of Chemistry, 90 Bader Lane,Kingston, ON K7L 3N6, Canada (20jjec@queensu.ca).

The increasing prevalence of 3D-printed firearms composed of polymer-based materials presents a significant challenge for forensic examination, as conventional ballistic identification methods rely on reproducible metallic toolmarks that are often absent or poorly defined in these systems. While polymer transfer to bullets and cartridge cases has been reported, robust analytical methods for non-destructive, spatially resolved, multi-element characterization of polymer surfaces remain scarce. Liquid microjunction (LMJ) sampling coupled with inductively coupled plasma mass spectrometry (ICPMS) enables localized surface extraction with direct, sensitive multi-element detection. In this work, LMJ-ICPMS is systematically evaluated as an approach for the elemental characterization of polymer materials relevant to 3D-printed firearm components. Preliminary results demonstrate that intact polymer surfaces produce reproducible transient signals associated with inorganic additives and pigments, highlighting the potential for differentiation between polymer types under controlled conditions. Elemental profiling further provides access to trace manufacturing signatures not readily captured by conventional molecular spectroscopic techniques. A redesigned LMJ probe enhances microjunction stability and improves signal consistency, enabling more controlled and reproducible measurements. Ongoing work focuses on reproducibility, signal normalization, and method optimization. These results establish LMJ-ICPMS as a promising non-destructive approach for forensic characterization of polymer-based evidence.

T830613

OPTOPLASMONICS AND DEUTERIUM ISOTOPIC LABELLING FOR RAPID ANTIBIOTIC SUSCEPTIBILITY TESTING. **Malama Chisanga***[1]; Ryma Boudriesa [1]; Claudele Lemay-St-Denisb [2]; Xinran Weic [3]; Yuzhang Liang [3]; Mengdi Lu [3]; Wei Peng [3]; Joelle N. Pelletier [2]; Jean-Francois Masson [2]. [1] Department of Chemistry, Dalhousie University, Coburg Road, Halifax, NS, B3H 4R2, Canada; [2] Department of Chemistry, Institut Courtois, Québec Centre for Advanced Materials (QCAM); [3] Regroupement Québécois sur les Matériaux de Pointe (RQMP), and Centre interdisciplinaire de recherche sur le cerveau et l'apprentissage (CIRCA), Université de Montréal, CP 6128 Succ. Centre-Ville, Montréal, Québec, H3C 3J7, Canada; [3] College of Physics, Dalian University of Technology, Dalian, 116024, China (malama.chisanga@dal.ca).

Antimicrobial resistance (AMR) is considered the silent pandemic of the 21st century, directly implicated in over 1.2 million deaths globally each year. Existing gold-standard tools for AMR are slow and time consuming, leaving physicians with no choice but to prescribe broad-spectrum antibiotics, which in turn exacerbates AMR. This necessitates the development of new tools for rapid drug resistance profiling to guide judicious therapeutic interventions. Plasmonic sensing based on surface-enhanced Raman scattering (SERS) readout has emerged as a potential analytical tool for rapid bacterial phenotyping and antibiotic susceptibility testing (AST). We have developed a novel strategy that combines fibre nanosensor-driven plasmonic sensing with deuterium isotopic probing

(DIP) and machine learning to enable rapid and unequivocal AST. This optoplasmonics-DIP strategy completed bacterial AST in 2 h, orders of magnitude faster than conventional methods. In this talk, I will discuss our efforts to develop (1) highly curved nanosensors from pre-synthesised plasmonic nanoparticles and polymer-templated glass fibres, and (2) heavy water-augmented DIP to uncover the kinetics of deuterium uptake by bacteria and molecular patterns underlying the drug resistance phenotype. Given that DIP can be readily integrated into the standard AST workflow, our optoplasmonics and DIP tools are well-positioned for clinical

T841016

MULTIELEMENT DETECTION OF METAL-BASED NANOPARTICLES IN BIOLOGICAL FLUIDS BY ADVANCED SINGLE-PARTICLE ICP-MS. **Ciprian M. Cirtiu***. Institut national de santé publique du Québec (INSPQ), 945 Av. Wolfe, Québec, QC, G1V 5B3, Canada. (ciprian-mihai.cirtiu@inspq.qc.ca).

Metal-based nanoparticles (NPs) are increasingly used in industrial, biomedical, and consumer applications, raising concerns about human exposure through environmental and dietary pathways. Following internalization, nanoparticles may circulate in biological fluids, interact with cellular systems, and undergo physicochemical transformations. Reliable analytical approaches are therefore required to detect and characterize heterogeneous nanoparticle populations in complex biological matrices. In this work, advanced single-particle inductively coupled plasma mass spectrometry (sp-ICP-MS) was evaluated for the detection and multielement characterization of metallic and metal oxide nanoparticles in biological fluids. Recent developments in high-speed data acquisition enable the simultaneous measurement of multiple elemental signals originating from individual particles within a single analytical run. Optimized sp-ICP-MS protocols were applied to characterize environmentally and biologically relevant nanoparticles, including Au, Ag, TiO2, CeO2, SiO2, Pb, Pd and CuO, in aqueous solutions and biological matrices. Particle size distributions and number-based concentrations were assessed while addressing matrix-related background signals, particle aggregation, dissolution, and spectral interferences using surfactant stabilization and collision/reaction cell strategies. Method validation for biological matrices was performed following ISO/IEC 17025 principles, including evaluation of selectivity, sensitivity, precision, and trueness under matrix-relevant conditions.

T92087

(VIRTUAL) MATRIX EXTENSION OF FDA METHOD EAM 4.11 (ARSENIC SPECIATION IN RICE AND RICE PRODUCTS USING HPLC-ICP-MS DETERMINATION) FOR INFANT FORMULA. **Sean Conklin***. Office of Chemistry and Toxicology, Office of Analytical Operations and Applied Science, Human Foods Program, U.S. Food and Drug Administration, 5001 Campus Drive, College Park, MD 20740, USA (Sean.Conklin@fda.hhs.gov).

FDA's Human Foods Program, through the Closer to Zero and Operation Stork Speed initiatives, emphasizes reduction of dietary exposure to contaminants to as low as possible, while maintaining

access to nutritious foods including infant formula. Toxic elements, including arsenic, are a focus of these initiatives. Since toxicity varies widely among arsenic species, it is important to identify which arsenic forms are present to appropriately evaluate potential health effects. FDA Elemental Analysis Manual (EAM) 4.11 was multi-laboratory validated for the analysis of 4 arsenic species in rice and rice products using high performance liquid chromatography inductively coupled plasma-mass spectrometry. In this work, EAM 4.11 was extended to include infant formula. Method performance was evaluated for accuracy and precision in milk-, soy-, and goat milk-based infant formula fortified at 5, 10, and 20 ng/g, with analyses performed in duplicate. The process and results of this work will be discussed in this presentation.

T930113

ONLINE APPLICATION FOR LIQUID CHROMATOGRAPHY SYSTEM PERFORMANCE ASSESSMENT VIA OPTIMIZABLE MACHINE LEARNING ANALYSES OF PRESSURE TRACE MEASUREMENTS. **Miroslava Cuperlovic-Culf***[1,3]; Irina Alecu [1,2]; Anuradha Surendra [3]; Thao Nguyen-Tran [1,2,4]; Evan Bushnik [1,2]; Caitlin Fowler [3]; Steffany A.L. Bennett [1,2,4]. Department of Biochemistry, Microbiology, and Immunology, University of Ottawa, Ottawa, ON, K1H 8M5, Canada [1]; Neurolipidomics Laboratory, uOttawa Brain and Mind Research Institute, University of Ottawa, Ottawa, ON, K1H 8M5, Canada [2]; Digital Technologies Research Centre, National Research Council of Canada, 1200 Montreal Road, Ottawa, ON, K1A 0R6, Canada [3]; Department of Chemistry and Biomolecular Sciences, Centre for Catalysis Research and Innovation, University of Ottawa, Ottawa, ON, K1N 6N5, Canada [4]. (Miroslava.Cuperlovic-Culf@nrc-cnrc.gc.ca).

Liquid chromatography (LC) hyphenated to molecular species detection systems such as mass spectrometer (MS) or Nuclear Magnetic Resonance (NMR) is often an essential component of lipidomics, metabolomics or proteomics analysis of highly complex samples. We are presenting novel approaches with several Machine Learning (ML) methods for automated analysis of LC pressure profiles providing information about possible problems in the LC performance or experiment characterization. Analysis of LC pressure profile properties and anomalies presents unique challenges where sensor streaming data comes in segments of possibly different length and characteristics due to method changes. Computational protocols presented here are built to explore overall pressure trace as part of routine measurements. We provide computational solutions for three different use cases including: a) re-labelling of LC experiments based on historical data providing information about any sample or method labelling errors; b) test quality of the run by comparing current experiment to prior experiments and c) provide unsupervised information about the experiments' similarities based on pressure traces. Analyses combines advanced ML applications for supervised, unsupervised and change point detection with pressure trace appropriate preprocessing, in all cases automatically optimized for users' specific data and analytical questions. Methods will be showcased using a set of experimental pressure measurements obtained as part of a normal instrument use for a 6-month period. User-friendly online implementation will be demonstrated at the conference.

T831011

BUILDING THE FOUNDATION FOR ENVIRONMENTAL NANOBIOGEOCHEMISTRY: SCOPE, PROGRESS, AND FRONTIERS. **Chad W. Cuss***[1]; Salani U. Fernando [1]; Claire M. Churchill [1]; Lakshman W. Galagedara [1]; Manokararajah Krishnapillai [1]; [1]; Isabelle A. M. Worms [2]; Vera Slaveykova [2], M. Tharaud [3]; Marc F. Benedetti [3]; Houssame-Eddine Ahabchane [4]; Madjid Hadioui. [1]; Salani U. Fernando [1]; Claire M. Churchill [1]; Lakshman W. Galagedara [1]; Manokararajah Krishnapillai [1]; [1]; Isabelle A. M. Worms [2]; Vera Slaveykova [2], M. Tharaud [3]; Marc F. Benedetti [3]; Houssame-Eddine Ahabchane [4]; Madjid Hadioui [4]; Kevin J Wilkinson [4] Michaela Schmitz [5]; Roland Drexel [5]; Florian Meier [5]; Agil Azimzada [6]; Björn Meermann [6]. [1] Laboratory for Environmental and Analytical Nanogeochemistry, Memorial University of Newfoundland, Canada; [2] Département F.-A. Forel des sciences de l'environnement et de l'eau, Université de Genève, Switzerland; [3] Université Paris Cité – Institut de Physique du globe de Paris, CNRS, F75005 Paris, France; [4] Biophysical Environmental Chemistry Group, Université de Montréal, Montréal, Canada; [5] Postnova Analytics GmbH, Landsberg, Germany; [6] Federal Institute for Materials Research and Testing (BAM) – Division 1.1 – Inorganic Trace Analysis (ITALab), Berlin, Germany. (ccuss@mun.ca).

T81084

Environmental nanobiogeochemistry is a new research area focusing on environmental geochemistry at the nanoscale. Initial work focuses on the development, application and refinement of specialized methods for environmental nanoanalysis, including single particle ICP-time-of-flight-MS (spICP-TOFMS) and asymmetric flow field-flow fractionation coupled to ICP-MS (AF4-ICPMS). These approaches provide complementary information about the composition, forms and distributions of particles and colloids that are associated with minerals and contaminants in natural nanoparticle systems (NNPS), in turn facilitating their robust characterization, connection to ecosystem roles, and assessing the impacts of disturbances. After briefly introducing the scope and aims of environmental nanobiogeochemistry, this presentation will report on recent applications of spICP-TOFMS and AF4-ICPMS by students in the Laboratory for Environmental and Analytical Nanogeochemistry in NL, Canada, and beyond. This includes the initial development of an NNPS standard and subsequent interlaboratory comparisons with international collaborators, and the combined application and comparison of spICP-TOFMS and AF4-ICPMS to investigate solutions extracted from various soils using tension lysimeters. We will then return to the goals of environmental nanogeochemistry to consider next steps, challenges, and frontiers.

P750126

PROTEOMIC CHANGES DURING RESOLUBILIZATION OF ACETONE–SALT PRECIPITATED PROTEINS REVEALED BY LC–MS. **Ziheng Dang***; Chukwuemeka Edeh, Alan A Doucette. Department of Chemistry, Dalhousie University, Halifax, NS B3H 4R2, Canada (ziheng.dang@dal.ca).

Protein precipitation using organic solvents is widely used for sample cleanup prior to mass spectrometry (MS), with acetone–salt systems offering high recovery and simplicity. However, efficient resolubilization of protein pellets under MS-compatible conditions remains a major challenge, often leading to sample loss and reduced analytical sensitivity. Previous work from our group demonstrated that the addition of different salts significantly affects acetone-induced protein precipitation, influencing not only recovery but also the composition of complex proteomes. [1] In this study, building on prior precipitation studies, we focus on factors governing protein resolubilization following acetone precipitation. Using hemp (Cannabis sativa) extract and aqueous extracts of bovine liver tissue as model systems, proteomic analysis by LC–MS was performed before and after resolubilization to assess differences in protein recovery. In addition, metal content associated with precipitated pellets formed in the presence of different cationic salts was quantified by MP-AES to further elucidate mechanisms of salt-assisted acetone precipitation. These results provide practical insights into optimizing protein recovery and improving reproducibility in proteomic sample preparation.

T81021

DEGRADABLE POLYESTERS FOR IMMUNOREGULATORY METABOLITE DELIVERY. **Davenport Huye***[1]; Locke [2]. Department of Microbiology & Immunology, Faculty of Medicine, Dalhousie University, Halifax, NS B3H 4R2, Canada. School of Biomedical Engineering, Faculties of Medicine [1]; Engineering, Dalhousie University, Halifax, NS B3H 4R2, Canada, Nova Scotia Health, Halifax, NS B3S 0H6 Canada [2]. (l.davenporthuyer@dal.ca).

Metabolites derived from central carbon metabolism play a critical role in maintaining immune homeostasis by engaging intrinsic feedback mechanisms that restrain pro-inflammatory signaling. In chronic inflammatory and fibrotic diseases, these endogenous regulatory pathways are frequently dysregulated or insufficient to resolve inflammation, motivating growing interest in metabolite-based immunotherapies. However, direct delivery of small-molecule metabolites remains fundamentally limited by high polarity, short biological half-life, the need for high local concentrations, and predominantly intracellular modes of action, collectively hindering sustained and therapeutically effective immune modulation. In this talk, I will describe a polymer-based approach to immunoregulatory metabolite delivery using degradable polyesters built from metabolite-derived monomers. Rather than encapsulating or conjugating small molecules, carboxylic acid metabolites are incorporated directly as structural monomers within the polymer backbone. In these systems, endogenous metabolites such as the di-carboxylate itaconate comprise up to ~50% of the backbone by mass, transforming the material itself into the therapeutic agent rather than a passive delivery

vehicle. Metabolite release is governed by fundamental polymer synthesis and degradation principles. I will describe how co-monomer selection, monomer stoichiometry, and polymerization conditions are used to tune molecular weight, physicochemical properties, and degradation kinetics, thereby defining both material performance and therapeutic output. This structure property function relationship enables rational matching of release profiles to the temporal dynamics of chronic inflammatory niches. The synthetic versatility of this platform supports fabrication across multiple material architectures, including resorbable bulk materials suitable for injection, implant-associated coatings, and microparticle systems for localized delivery. Across these formats, degradation-driven metabolite release preserves long-term material function while providing sustained immunoregulatory signaling at the tissue interface. By integrating intrinsic immunometabolic regulation with polymer chemistry, this work establishes a localized, carrier-free delivery strategy to restore dysregulated immune feedback.

P750737

CHARACTERIZING THE STRUCTURE AND SELF-ASSEMBLY OF A HYDROPHOBIN FROM PHANEROCHAETE CARNOSA. **David Langelaan***;Calem Kenward ; Raymond He. Department of Biochemistry & Molecular Biology, Dalhousie University, Halifax, NS (dlangela@dal.ca).

Hydrophobins are small, secreted proteins that play vital roles in the growth and development of filamentous fungi. They have the unusual ability to accumulate at hydrophobic-hydrophilic interfaces, where they self-assemble into larger structures called rodlets. These rodlets coat surfaces such as fungal spores, making them extremely water repellent. Hydrophobins have been used to modify surfaces to prevent fouling or biofilm formation, as drug delivery agents, as biosensors, and to make hydrophobic surfaces more biocompatible. It is necessary to understand the structure and self-assembly mechanisms of hydrophobins so that their properties can be controlled and applied. This project focuses on PC1, a model hydrophobin from Phanerochaete carnosa. We used NMR spectroscopy to determine the structure of PC1, atomic force microscopy to observe rodlet morphology, and thioflavin-T based assays to observe a pH-dependent ability for PC1 to self-assemble. NMR-monitored pH titrations suggest that there are no major structural changes, but that some regions of PC1 are protonated upon pH changes. These results shed light on the structural conservation of hydrophobins and hints at potential mechanisms of self-assembly.

P750127

INFORMATION-DEPENDENT ACQUISITION ENHANCED-PRODUCT ION SCAN ENABLES ELUCIDATION OF LIPIDOMIC SIGNATURE IN PLASMA OF PATIENTS WITH CEREBRAL SMALL VESSEL DISEASES (CSVD). **Esther Dazogbo***[1,2]; Thao Nguyen-Tran [1,2]; Eric Smith [3]; Steffany A. L. Bennett [1,2]. Neurolipidomics Lab, India Taylor Lipidomic Research Platform, and Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, ON, Canada K1N 6N5 [1];

Ottawa Institute of Systems Biology, Department of Biochemistry, Microbiology and Immunology, University of Ottawa, Ottawa, ON, Canada K1H 8M5 [2]; Department of Clinical Neurosciences, University of Calgary, Calgary, AB, Canada [3]. (edazo053@uottawa.ca).

Information-Dependent Acquisition (IDA) is a tandem mass spectrometry (MS/MS) tool which bridges a survey scan and subsequent experiment to select specific ions for further qualitative analysis via specified signal threshold criteria. We developed an analytical protocol utilizing IDA by combining Multiple Reaction Monitoring (MRM) as a survey scan for quantification and Enhanced Product Ion (EPI) scans for qualitative structural information. We applied this protocol to our lipidomic pipeline to study aberrant lipid metabolism in the plasma of patients with vascular cognitive impairment (VCI) due to cerebral small vessel diseases (cSVD). Our lipidomic pipeline defines Lipid Identification Level based on annotation score by liquid chromatography retention time and assignment score by IDA-EPI experiment. Based on this, our pipeline quantified and identified molecular species of cerebrosides, ceramides, sphingomyelins, glycerophosphocholines and glycerophosphoethanolamines in patients' plasma and cerebrospinal fluid, with identification level assigned to each. This work provides confidence and clarity to lipidomic profiling pipeline, and efficacy for identifying lipid biomarkers predisposing cSVD individuals to risk of accelerated cognitive decline.

T81019

MONITORING CRITICAL QUALITY ATTRIBUTES ON LARGE MOLECULE THERAPEUTICS USING BIOZEN LC SOLUTIONS. **Saba Dehghani-Tafti***; Vikram Shenoy. Phenomenex, 411 Madrid Avenue, Torrance, CA 90501 USA (rra016@mail.usask.ca).

Comprehensive characterization of Critical Quality Attributes (CQAs) is essential to ensure the safety, efficacy, and consistency of biotherapeutics throughout development and manufacturing. This presentation will highlight integrated LC and LC-MS workflows for monoclonal antibody and protein therapeutic characterization using the bioZen™ Bio Series column portfolio. Applications will include SEC for size variants and aggregates, CEX-HPLC for charge variant analysis, peptide mapping for PTM identification and sequence confirmation, RP-HPLC-MS for intact mass and subunit analysis, and HILIC glycan mapping for glycosylation profiling. TTogether, these orthogonal approaches provide a robust framework for comprehensive CQA assessment across biopharmaceutical development, process optimization, and quality control workflows.

T81083

IDENTIFICATION OF ARSENOLIPIDS IN MARINE STANDARD REFERNCE MATERIALS BCR-627 AND DOLT-5. **Amrika Deonarinea***;Jocelyn Fostera; Shubhra Bhattacharjeea; Miguel Chacon Teranb; Michael Findlaterb; Jeremy Bailooc; Stacey Louied. Department of Chemistry & Biochemistry, Texas

Tech University, 1204 Boston Avenue, Lubbock, TX 79409, United States (amrika.deonarine@ttu.edu).

Arsenolipids are a group of fat-soluble arsenic-containing compounds with potential toxicological consequences. However, research on their health effects remains limited. Accurate identification and quantification of arsenolipids in foods is challenging due to the complexity of arsenolipid structures in food matrices and the lack of standard reference materials (SRMs). To address these challenges, we present a workflow for identifying arsenolipids in two commercially available SRMs: dogfish liver (DOLT-5) and tuna fish (BCR-627). Samples were extracted using hexane and dichloromethane/methanol and analyzed by reverse-phase high-performance liquid chromatography (LC)–inductively coupled plasma mass spectrometry and LC coupled with electrospray ionization quadrupole time-of-flight mass spectrometry (LC–ESI–QTOF–MS). A precursor library of reported arsenolipids was used to aid compound identification, which was confirmed by mass fragmentation, retention time matching, and mass error evaluation. Data was processed with MassHunter Qualitative Analysis software, applying a mass match tolerance of ±10 ppm for target screening, fragment mass filtering with ±0.5 m/z tolerance, and a minimum confidence score of 70. AsHC332 and AsFA362 were found in tuna and AsFA486, AsFA502, and pentylarsonic acid in dogfish liver. These SRMs are potential candidates for arsenolipid-certified reference materials, and the reported workflow supports improved reproducibility in arsenolipid-related research.

T82055

A TRANSISTOR GATED ELECTROCHEMICALLY AND ACTUATED BY QUANTUM MECHANICAL EXCHANGE DURING REDOX AND BONDING. **Al-Amin Dhirani***[1,2,3]; Xiaoyang Chen [1]. [1] Department of Physics; [2] Department of Chemistry; [3] Department of Materials Science and Engineering, University of Toronto, Canada. (a.dhirani@utoronto.ca).

Modern computing has at its heart the field effect transistor (FET) - an elegant 3-electrode device that enables switching. Application of a gate voltage classically charges the channel and actuates resistance changes. Here, we present “quantum charge exchange transistors” (qCETs) that combine FET with electrochemistry. We use a thin metal film as the working electrode (CET channel) and monitor its resistance during cyclic voltammetry. The metal film exhibits remarkable resistance peaks during metallocene - metal film redox charge exchange. Multiple evidence, including various measurements, kinetic modelling and density functional theory calculations are consistent with a multi-step redox pathway that includes the formation/destruction of a hybrid metallocene + metal state that actuates the observed resistance changes. q-CET is also actuated by thin film – analyte bonding, allowing real-time measurements of kinetics with submonolayer sensitivity. These results provide important new insight into mechanisms involved in quantum charge exchange; conversely, they point to important applications of CET as means for probing and potentially exploiting such

phenomena, including providing a window into catalytic processes in-situ, in-operando and in real time and sensing species with low limits of detection.

T830213

NANO-BIOMATERIALS FOR DIAGNOSTICS, THERAPEUTICS AND PREVENTING SPREAD OF INFECTIOUS DISEASES. **Tohid F. Didar***. School of Biomedical Engineering, McMaster University, Hamilton, Ontario, Canada (didart@mcmaster.ca).

The biological/non-biological interface system is an important cornerstone for the fabrication of a wide range of biomedical devices. Platforms as diverse as lab-on-chip and point-of-care diagnostics, 3D tissue culture scaffolds, organs-on-chips, implants and antimicrobial surfaces all rely on the effective interaction of cells and/or bio-recognition elements (proteins/peptides, enzymes, oligonucleotides, etc.) with non-biological surfaces. Design and engineering of micro/nano patterned interfaces provide powerful tools to study biological phenomena at micro and nano scale and to develop novel technologies for diagnostics, therapeutics and preventing the spread of infectious diseases. I will present an overview of our research on design and development of transformative nanomaterials and their integration into in vitro systems such as lab on chip devices, flexible sensing interfaces, smart food packaging and antimicrobial and pathogen repellant coatings as well as in vivo applications to develop efficient medical devices such as injectable hydrogels, anti-thrombogenic and antimicrobial catheters, vascular grafts and implants.

T92055

ELECTROCHEMILUMINESCENCE OF A GRAPHENE QUANTUM DOT MODEL MOLECULE WITH ATOMIC PRECISION AND TRANSLATABLE ENERGY LEVELS. **Zhifeng Ding***; Ziying Zhan. Department of Chemistry, Western University, 1151 Richmond St, London ON N6A 5B7 (zfding@uwo.ca).

The electrochemistry and electrochemiluminescence (ECL) of a water-soluble atomically precise graphene quantum dot model molecule, WAGQD-C96, were studied using an absolute-quantification strategy for the first time. Absolute ECL efficiency was determined to be 17.1 ± 0.9% under optimized conditions without the use of reference luminophores, which is the highest so far of a variety of luminophores. WAGQD-C96 exhibits five well-resolved and evenly spaced (ΔV = 0.20 ± 0.05 V) reduction peaks and oxidation waves each in differential pulse voltammograms (DPVs), with highly reversible and reproducible reduction reactions due to its atomically defined electronic structure. Density functional theory (DFT) calculations explained the ten redox peaks in the DPVs, enabling a direct link between molecular-level electronic configuration and the redox behaviors. Spooling ECL spectroscopy reveals distinct dynamic emission features. Analysis of the accumulated spectra over a cyclic voltammetry (CV) run shows composite bands at 650 and 694 nm, attributing

to (0,1) and (0, 2) vibronic transitions and a near-infrared band at 810 nm arising from aggregation-induced emission (AIE).

T940116

PROPOSAL FOR A NATIONAL PROGRAM TO DELIVER ADVANCED ANALYTICAL CHEMISTRY EDUCATION. **Alan Doucette***. Department of Chemistry, Dalhousie University, Halifax, NS, B3H 4R2, Canada (alan.doucette@dal.ca).

ICASS 2026 brings together the very best analytical researchers, trainees and industry leaders. Individually, our work is continuously expanding the scope of analytical science as our advances demonstrate new possibilities for chemical measurement. Collectively, our knowledge highlights the diversity of chemical analysis, and benefits the many trainees and future leaders of our field. The real question is – how can we pass on that knowledge and provide the best training for these future scientists? The educational landscape is rapidly changing, as students can now access knowledge from a number of sources − some fantastic, others questionable. Unfortunately, most educators realize their limitations in terms of personal expertise, and personal time commitment. In short, we can't cover everything, as much as we wish we could. But we don't have to! This presentation proposes a national network of analytical educators who can come together to provide the best training opportunities for future scientists. And don't worry – your attendance at this presentation won't tie you into additional teaching commitments! But I would sincerely appreciate your thoughts on a shared teaching program in the analytical sciences.

T740119

PROTEOME-WIDE SEROLOGY FOR VIRAL DIAGNOSTICS AND THE DISCOVERY OF HIGH-AFFINITY HUMAN ANTIBODIES. **Andrei Drabovich***; Zoe Turner; Yasmine Rais; Weize Tang. Department of Laboratory Medicine & Pathology, University of Alberta (drabovic@ualberta.ca).

Human serum antibodies comprise a highly diverse mixture of isotypes, subclasses, and clonotypes that collectively shape the immune response. Informative sequencing of polyclonal antibodies by mass spectrometry remains a challenge due to the lack of universal sequence-matching databases. Novel assays for measuring antigen-specific antibodies have practical implications for serological diagnostics of infectious diseases. Here, we developed Proteome-Wide Serology assays aimed at characterization of the full-scale depth and diversity of human polyclonal antibody response. High-throughput antibody enrichments using recombinant viral antigens were followed by untargeted and targeted mass spectrometry assays (timsTOF Ultra 2, QTRAP 6500+). Proteome-Wide Serology assays were validated with over 20 recombinant antigens of Influenza A, RSV, SARS-CoV-2, and their variants. Blood serum samples from over 500 individuals were analyzed. Antigen-specific IgG1 (~1-3 µg/mL) were elevated across all viral infections, while RSV elicited a distinct immune response. Repertoire profiling of heavy-chain variable regions revealed patient-specific patterns and frequent use of a small subset of IGHV genes in polyclonal response. Proteome-Wide Serology facilitates

rational design of serology diagnostics for viral infections and characterization of polyclonal antibody mixtures for selection and sequencing of high-affinity clones.

P750732

PRECISE SIDE CHAIN ROTAMERIC CONSTRAINTS APPLICATION TO NMR STRUCTURE DETERMINATION. **Thomas Dumont***. University of Alberta, Department of Biochemistry,114-11450 80 Avenue, Edmonton, AB T6G 2X3, Canada (twdumont@ualberta.ca).

Conventional NMR chemical shift-based dihedral angle restraints and distance restraints from nuclear Overhauser enhancements (NOEs) are insufficient for defining many side chain positions in a protein. We have developed robust methodology for determining precise side chain dihedral angles for protein residues with rigid side chains, and rotamer populations for flexible side chains. We distinguish between rigid and mobile residues using1H-NMR transverse relaxation rates. We then fit quantitative J coupling data (3-bond J couplings for N-HB, CO-HB, and HA-HB) to the appropriate model. We apply our methodology on a 131-residue chimeric protein construct of human cardiac troponin complex. We were able to obtain excellent side chain data for all structured residues in our protein construct. Most side chains are mobile, being able to access at least two major side chain rotameric states. 36/131 residues were deemed to have a single rotameric state that we restrained to +/- 10 degrees. 9 residues were found to be constrained to a single completely wrong rotameric state without dihedral restraints. The combined use of1H relaxation and quantitative J coupling analysis leads to NMR structure determinations of unprecedented quality in terms of side chain structure determination in structure and dynamics.

T81052

MECHANISTIC INSIGHTS INTO FERROCENE-MEDIATED OXIDATIVE ELECTROPLATING. **E. Bradley Easton***; Olena V. Zenkina; Marjan Saeidi; Ghazaleh Donyapeyma; Yelyzaveta V. Antsybora, Iraklii. Ebralidze Electrochemical Materials Lab, Faculty of Science, Ontario Tech University, Oshawa, Ontario, Canada L1G 0C5 (brad.easton@ontariotechu.ca).

Covalent modification of electrode surfaces by redox-active molecules is central to the design of functional materials for energy and electronic applications. Electrografting is particularly attractive because the applied potential directly governs the generation of reactive intermediates and film growth. Ferrocene (Fc) units are widely used as electrochemically reversible redox probes, yet are generally assumed to be chemically inert toward surface coupling. Here we demonstrate an unexpected oxidative electrografting mechanism in which pendant Fc groups act as the active grafting site. During cyclic voltammetry (CV) of iron terpyridine–ferrocene complexes, $Fe(tpy\text{-}Fc)_2^{2+}$ (tpy = 2,2':6',2"-terpyridine), in acetonitrile electrolyte, oxidation of the Fc moieties leads to the formation of a persistent, electroactive surface film. CV profiles indicated oxidative electrografting

occurs through successive oxidation of the metal centers. Surface confinement is confirmed by X-ray photoelectron spectroscopy (XPS), and modified indium tin oxide (ITO) electrodes exhibit rapid, reversible electron transfer in fresh electrolyte. We have successfully extended this method to $Ru(tpy\text{-}Fc)_2 2+$ and also demonstrated film growth on high-surface-area carbon electrodes, highlighting the method's versatility. Mechanistic insights into film growth are discussed, along with their implications for the design of advanced electrode architectures for sustainable energy and smart technologies.

T840117

IMPROVING TRACE-LEVEL DETECTION OF PYOCYANIN ACROSS ENVIRONMENTAL AND BIOLOGICAL MATRICES VIA HPLC COLUMN OPTIMIZATION AND MS PARAMETER TUNING. **Chukwuemeka Edeh***; Alan Doucette. Department of Chemistry, Dalhousie University, Halifax, NS, B3H 4R2 (bf638776@dal.ca).

Pyocyanin, a redox-active metabolite, is a clinically and environmentally relevant biomarker whose detection at trace levels in complex matrices remains challenging. This work presents combined chromatographic and mass spectrometric strategies to enhance detection sensitivity and signal response. Isocratic HPLC optimization using a commercially C18 column established retention characteristics and yielded a limit of detection (LOD) of 0.5 μM. To improve sensitivity, a narrow diameter C18-packed column was packed in house, resulting in enhanced analyte interaction and improved LOD to 0.1 μM. The method was evaluated in pyocyanin-spiked matrices, including simulated sweat water, harbor water, and simulated wound fluid, to assess matrix effects and robustness. Complementary mass spectrometric optimization is ongoing, including variation of sheath gas, auxiliary gas, capillary voltage, spray voltage, and capillary temperature, which further improved ionization efficiency and signal intensity demonstrating further enhancement in detection of trace-level of pyocyanin.

T81093

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

The presence of Mn in drinking water has shown to have negative neurological effects on children, representing a critical public health concern requiring the development of novel point-of-use tools for water quality monitoring. Although treatment may be in place, trace levels of Mn leaving the treatment plant can accumulate within the distribution system as reservoirs and can be released back into the bulk drinking water at levels exceeding Health Canada's maximum allowable

concentration (based on total Mn).1,2 Traditional spectroscopic techniques for Mn monitoring are not practicable for on-site detection due to their size and cost. Alternatively, electrochemical methods, which are promising for on-site monitoring are limited to the measurement of dissolved species.2,3 This work explores digestion procedures for insoluble Mn to prepare samples for electrochemical detection.2 Parameters including pH, digestion time, Mn concentration and the presence of common contaminants are considered. This research will allow for all forms of Mn to be monitored on-site, representing a breakthrough in Mn management.

T91084

VITAMIN B12 SURVEY OF INFANT FORMULA FROM THE U.S. MARKET. **Jordan Escavage***. Oak Ridge Institute for Science and Education, Oak Ridge, TN 37831, USA. Mesay M. Wolle, U.S. FDA, 5001 Campus Drive, College Park, MD 20740, USA (Jordan.escavage@fda.hhs.gov).

Vitamin B12 is an essential, water-soluble micronutrient critical for brain function and red blood cell formation. Dietary intake is the only source of B12, and therefore infant formulas are fortified with B12 where formula may be the sole source of nutrition. It is critical that infant formula products contain sufficient B12 to support infant development. The U.S. FDA recently developed and single-lab validated a method to quantify B12 across food products including infant formula using HPLC-ICP-MS. In this work, a partial market basket survey was conducted at the U.S. FDA to measure vitamin B12 in infant formulas available on the U.S. retail market. One hundred and twenty-six formulas were analyzed and categorized according to brand, manufacturer, product form, formula type, and protein source. The survey results indicate that infant formulas for sale in the U.S. market all meet the minimum vitamin B12 requirement set by the U.S. Code of Federal Regulations and other international regulatory bodies. Measured levels of vitamin B12 ranged between 152-462% of the corresponding label claim in tested products. Trends in vitamin B12 overages point mainly to an association with product brand.

P750644

NEW STRATEGIES FOR SUSTAINABLE CHEMICAL FEEDSTOCKS: PHOTOCATALYTIC AMMONIA GENERATION. **Scarlett Evans***; Geniece Hallett-Tapley. St. Francis Xavier University, Department of Chemistry, 5009 Chapel Square, Antigonish, NS B2G 2W5, Canada. (x2023aqd@stfx.ca).

Due to the current climate crisis, the development of net-zero alternative fuel technologies has become a global priority. Hydrogen (H_2) production and ammonia (NH_3) synthesis are particularly attractive targets; however, conventional industrial methods remain highly energy-intensive and greenhouse gas emitting. Ammonia synthesis via the fossil-fuel-powered Haber–Bosch process accounts for ~2% of global energy consumption and produces approximately 500 Mt of CO_2 annually, a burden further compounded by emissions from H_2 production. Improving the

sustainability of this globally critical agricultural process is of high societal importance. Moreover, nitrate contamination poses a significant challenge in regions of high agricultural activity due to demonstrated impacts on the environmental disruption of the environmental nitrogen cycle. Converting nitrate effluents into value-added feedstocks such as NH_3 offers a promising route toward environmental remediation. Previous work at StFX has demonstrated rapid, light-driven H_2 generation, using both artificial UV and solar light in the presence of copper-based nanocatalysts in and small polyols. Herein, an extension to this approach will be discussed, by employing polyethylene terephthalate (PET) microplastics as ethylene glycol precursors to promote nitrate reduction for sustainable ammonia production.

T830713

UNDERSTANDING RECOMBINANT ACINIFORM SILK FIBRILLOGENESIS THROUGH SOLID-STATE NMR SPECTROSCOPY. **Sara Evans***[1]; Lingling Xu [2]; Marie-Laurence Tremblay [2]; Anamika Sulekha [2]; Ivan Hung [4]; Frederic Mentink-Vigier [4]; Xiang-Qin Liu [2]; Jan K. Rainey [1,3]. [1] Dalhousie University, Department of Chemistry, Halifax, Nova Scotia, Canada; [2] Dalhousie University, Department of Biochemistry & Molecular Biology, Halifax, Nova Scotia, Canada; [3] Dalhousie University, School of Biomedical Engineering, Halifax, Nova Scotia, Canada; [4] National High Magnetic Field Laboratory, Tallahassee, Florida, USA. (sara.evans@dal.ca).

Female orb-weaver spiders produce up to seven protein-based silks with mechanical properties corresponding to their function. Spiders use aciniform silk to contain prey and line egg sacs, making it strong, extensible, and hence tough. To rationally design new silk-based materials with specific properties, a fundamental understanding of the molecular determinants of mechanical properties and how they arise during fibrillogenesis is required. In this work, aciniform constructs were recombinantly expressed using two NMR labelling schemes and processed into fibres through wet-spinning. Dipolar-assisted rotational resonance (DARR) solid-state NMR experiments reveal an interaction between glutamine and tyrosine that is not detectable in the solution-state NMR structure and has not been previously detected in any other spider silk. Furthermore, this experiment reveals secondary structuring within the fibre, providing insights into the molecular transitions that occur during fibrillogenesis and how sequence elements contribute to the fibre mechanics. To distinguish between inter- and intramolecular interactions, selectively 13C- and 15N-unlabelled proteins were expressed separately then combined for DARR and proton-assisted insensitive nuclei (PAIN) experiments. These experiments and the analysis of their resultant spectra are ongoing. This work augments our understanding of aciniform silk fibrillogenesis, paving the way for the engineering of new silk-based materials with tunable properties.

T82027

HANDHELD MULTISPECTRAL IMAGING CYTOMETER FOR IMMUNOYTOMETRY, IMMUNOASSAYS, SEROLOGY AND HEMATOLOGY ON SINGLE DROPLET SAMPLE VOLUMES. **Alan Fine***[1,2]. [1] Departments of Physiology & Biophysics, Pediatrics; School of Biomedical Engineering, Dalhousie University, Faculty of Medicine, Halifax, Nova Scotia Canada Alentic Microscience Inc., Halifax, Nova Scotia, Canada. (afine@alentic.com).

Critical in vitro diagnostic tests typically require tubes of blood, trained technologists and expensive specialized instruments; often hours or days are needed for return of results, and tests may simply be unavailable for many patients. To overcome these limitations, we developed a pocket-sized diagnostic platform device that use proprietary lensless transmitted light microscopy, specimen handling and artificial intelligence to carry out complete blood counts (CBC), multiplexed immunoassays, immunocytometry and serology in a matter of minutes on one droplet of whole blood. Pilot experiments were carried out to demonstrate the capabilities of these low cost devices in comparison to expensive standard instruments, and their ability to complex test panels combining multiple analytic modalities.Method comparison across the specimens obtained showed clinically useful correlations of all routine CBC measurands and of percent prevalence for lymphocyte subtypes between these devices and standard blood count instruments and fluorescence flow cytometers, respectively. Time from sample collection to results was less than 10 minutes for CBC and half an hour for immunophenotyping, vs more than 20 minutes and one hour for the respective standard instruments. Linearity and limits of detection on the compact system showed clinically useful performance.Though further development will be required, these proof-of-concept demonstrations demonstrate that these handheld device can move testing that has historically been restricted to central laboratories to remote or low-resource settings.

P751041

ANALYSIS OF MICROPLASTICS USING CRYOCELL LASER ABLATION SINGLE PARTICLE ICP-MS. **Andreas Limbeck***; Elias Foisner. TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, 1060 Vienna, Austria (elias.foisner@tuwien.ac.at).

Due to the increasing dissemination of microplastics in all environmental compartments, the need for reliable analysis methods is high. Over the last years, single particle ICP-MS has developed into an essential analytical tool for determination of particle size and number concentration [1,2]. However, conventional SP-ICP-MS of particle suspensions has drawbacks such as poor transport efficiency, occurrence of spectral interferences as well as sample storage and stability. These challenges can be overcome by employing laser ablation to desorb particles from a substrate surface intactly using low laser fluences and analyzing them via ICP-MS [3, 4, 5]. The aim of this work is to extend these advantages by using a cryocell to investigate particle-containing ice films. This allows

direct analysis of particles in their frozen suspension medium and offers significant benefits which will be presented in this contribution.

T831015

DETERMINATION OF NANOPARTICLE COMPOSITION USING LASER ABLATION SINGLE PARTICLE ICP-QMS. **Elias Foisner***; Andreas Limbeck. TU Wien, Institute of Chemical Technologies and Analytics, Getreidemarkt 9/164, 1060 Vienna, Austria (elias.foisner@tuwien.ac.at).

Due to the increasing dissemination of microplastics in all environmental compartments, the need for reliable analysis methods is high. Over the last years, single particle ICP-MS has developed into an essential analytical tool for determination of particle size and number concentration [1,2]. However, conventional SP-ICP-MS of particle suspensions has drawbacks such as poor transport efficiency, occurrence of spectral interferences as well as sample storage and stability. These challenges can be overcome by employing laser ablation to desorb particles from a substrate surface intactly using low laser fluences and analyzing them via ICP-MS [3, 4, 5]. The aim of this work is to extend these advantages by using a cryocell to investigate particle-containing ice films. This allows direct analysis of particles in their frozen suspension medium and offers significant benefits which will be presented in this contribution.

T92075

ENSEMBLES OF PROTEINS CONTAINING INTRINSICALLY DISORDERED REGIONS. **Julie Forman-Kay***[1,2]. [1] The Hospital for Sick Children, Molecular Medicine Program, 686 Bay St.,Toronto, ON M5G 0A4, Canada; [2] University of Toronto, Department of Biochemistry, 1 King's College Circle, Toronto, ON M5S 1A8, Canada (forman@sickkids.ca).

The structural characterization of proteins has focused on stable, folded elements. Yet, a third of residues in the human proteome are strongly predicted to be intrinsically disordered with two thirds of proteins containing significant intrinsically disordered regions (IDRs). AlphaFold and similar predictive tools misrepresent proteins containing IDRs, hindering biological intuition and hypotheses. Solution experimental data, including from NMR, SAXS and single molecule fluorescence, in combination with IDR-centric computational tools, can enable more realistic descriptions of ensembles of isolated disordered chains, full-length proteins having IDRs and folded domains, and complexes of IDRs with folded domains. Tools developed in collaboration with Teresa Head-Gordon (University of California Berkeley) will be discussed, together with applications, towards the goal of structural characterization of the full human proteome, including ensemble representations of IDRs.

T81084

TINY PARTICLES, BIG IMPACT: CRMS FOR VALIDATING SP-ICP-MS IN FOOD TESTING. **Zuzana Gajdosechova***[1]; Filip Gregar [1,2]; Monique E. Johnson [3]; Antonio R. Montoro Bustos [3]; Katrin Loeschner [4]. [1] Metrology Research Center, National Research Council Canada, 1200 Montreal Road, K1A 0R6, Ottawa, Ontario, Canada; [2] Palacky University Olomouc, Faculty of Science, Department of Analytical Chemistry, Czech Republic; [3] Chemical Sciences Division, Material Measurement Laboratory, National Institute of Standards and Technology, 100 Bureau Drive, Gaithersburg, MD 20899-1070; [4] Research Group for Analytical Food Chemistry, National Food Institute, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark (Zuzana.Gajdosechova@nrc-cnrc.gc.ca).

The accurate measurement of macro and trace elements in food is essential for ensuring safety, quality, and nutritional value. Certified reference materials (CRMs) play a key role in this process by providing standardized benchmarks that support the validation and comparability of analytical methods. Over the past two decades, the presence of nanoparticles (NPs) in food has received increasing attention, largely driven by advances in nanotechnology and its applications in food production and packaging. Among the available techniques, single particle inductively coupled plasma mass spectrometry (spICP-MS) has become the leading method for detecting and characterizing inorganic NPs in complex food matrices. Despite this progress, the suitability of existing CRMs, particularly those that may contain NPs, for supporting spICP-MS method development and validation has not been widely investigated. To address this gap, we examined CRMs certified for macro and trace elements in food as potential reference materials for spICP-MS. Selected CRMs were extracted using protocols published in the literature and analyzed for inorganic NPs, with results compared to previously reported data. Our findings showed strong agreement between published and newly acquired results, although significant software-dependent biases were observed. Overall, this work identified a suite of CRMs suitable for spICP-MS method validation and highlights the importance of considering data processing and sample homogenization effects, which may introduce discrepancies in reported results.

T91011

FROM SPECTRA TO SOLUTIONS: PROTEOMICS AT THE FOREFRONT OF FUNGAL INFECTION, IMMUNITY, AND RESILIENCE. **Justine R. Bissonnette***; Emmanuel C. Tolefe; Nikita E. Harvey; LindsayS. Cahill; Karl J. Jobst. Department of Chemistry, Memorial University of Newfoundland, 45 Arctic Ave., St. John's, Newfoundland and Labrador, Canada (jgeddesm@uoguelph.ca).

Fungal diseases impact the lives of millions of people across the globe ranging from superficial to systemic infections. Treatment options toward fungal diseases are limited given host cytotoxicity and availability, the emergence of new pathogens with intrinsic resistance and a heightened evolution toward resistant strains. To effectively combat fungal disease, my research team harnesses the cutting-edge power of mass spectrometry-based proteomics integrated with

computational biology. By identifying protein drivers of fungal disease, we can provide new biological insights across four pillars of research: i) Prevention, ii) Diagnostics, iii) Monitoring, and iv) Treatment. For prevention, we disrupt critical proteins and pathways to weaken the pathogen and prevent infection; for diagnostics, we define dual-perspective protein production signatures, spanning both host and pathogen, across spatial and temporal dimensions to enable precise diagnostic and prognostic insights. For monitoring and treatment, we explore host-pathogen interactions at the protein level, uncovering novel druggable targets essential for therapeutic innovation, and we combat antifungal resistance through protein targeting to restore the efficacy of existing antifungal drugs. Together, our integrated proteomics driven approach offers transformative solutions to fungal disease management with the goal of advancing global health initiatives.

T92088

ROUTINE DETERMINATION OF CR6+ AND CR3+ SPECIATION IN DRINKING WATER USING AGILENT ICPMS WITH METROHM ION CHROMATOGRAPHY INTEGRATION. **Yan Cheung***; Bastian Georg. Agilent Technologies Canada, 6705 Millcreek Dr., Unit 5, Mississauga, L5N 5M4, Ontario, Canada (bastian.georg@agilent.com).

Chromium is a naturally occurring transition metal element found in terrestrial and aquatic ecosystems. The predominating Cr species are trivalent Chromium Cr(III) and hexavalent Chromium Cr(VI). While Cr(III) is naturally found in the environment and even classed as an essential element to human health, toxic hexavalent Cr(VI) originates predominantly from industrial processes. Interconversion of Cr species is pH dependent and can occur in nature. Reliable determination of Cr concentration and Cr speciation is therefore crucial when assessing ecosystem health and monitoring the status of toxic Cr(VI). Here we show how Agilent ICPMS coupled to Metrohm Ion Chromatography systems can be used to obtain reliable Cr concentrations and also quantification of related Cr species in drinking water. We will show hardware setup, system interface setup as well as software integration into MassHunter.

T92017

INVESTIGATING THE EFFICIENCY OF ALGINATE-BASED ENZYME ENTRAPMENT IN HYDROGELS IN BOTTOM-UP PROTEOMICS COMPARING WITH THE TRADITIONAL METHODS. **Golfam Ghafourifar***. Chemistry Department, University of the Fraser Valley, 33844 King Rd., Abbotsford, BC V2S 7M8 (golfam.ghafourifar@ufv.ca).

In-solution digestion (ISD) has been widely used since the inception of proteomics. As reliable as ISD has proven to be over the past decades, it also carries several problems. In addition to inevitable sample loss, the trypsin:protein ratio is usually kept low to minimize enzyme autoproteolysis, which elongates digestion. Enzyme immobilization significantly reduces enzyme autoproteolysis by limiting

self interactions, which in turn allows for enhanced enzyme/protein ratios to significantly decrease digestion time. Alginate enzyme entrapment is a method of immobilizing proteolytic enzymes. We have developed a method to form an alginate hydrogel almost instantly. The enzyme then was injected into the center of the gel. The substrate was introduced to the top of the gel to diffuse, and the digests were then removed, and LC-MS/MS analysis was used to determine the amino acid sequence coverage of digestion. Using the entrapped trypsin, we have successfully digested various substrate with different complexity. The results then were compared with using the traditional in-solution digestion of the same samples looking at the peptides and amino acid sequences and showed no significant difference. We have also deployed our entrapped enzymes to various water bodies to analyze the protein contaminations of various locations.

P750123

METHOD-DEPENDENT DISCREPANCIES IN HYDROXYCHLOROQUINE BINDING TO SERUM ALBUMINS: A MULTIMODAL SPECTROSCOPIC AND COMPUTATIONAL STUDY. **Amirreza Gholami***[1,4]; Gholamreza Dehghan [1]; Sohrab Ahmadi-Kandjani [2,3]; Samaneh Rashtbari [1]; Alan A. Doucette [4]. [1] Laboratory of Biochemistry and Molecular Biology, Department of Biology, Faculty of Natural Sciences, University of Tabriz, Tabriz 5166616471, Iran; [2] Faculty of Physics, University of Tabriz, Tabriz 51663-165, Iran; [3] Research Institute for Applied Physics and Astronomy (RIAPA), University of Tabriz, Tabriz 51663-165, Iran; [4] Department of Chemistry, Dalhousie University, 6243 Alumni Crescent, Halifax, Nova Scotia, B3H 4R2, Canada (amirreza.gholami@dal.ca).

Hydroxychloroquine (HSQ) is an important therapeutic agent widely used in the treatment of malaria, autoimmune diseases, and inflammatory disorders. Understanding its interaction with serum albumins is essential for elucidating its pharmacokinetic behavior. In this study, the binding interaction of HSQ with human and bovine serum albumins (HSA and BSA) was investigated using a combination of spectroscopic techniques, surface plasmon resonance (SPR), and molecular docking approaches. SPR analysis confirmed the interaction between HSQ and serum albumins, revealing moderate binding affinity with temperature-dependent behavior. Fluorescence spectroscopy indicated that HSQ induces quenching of the intrinsic fluorescence of HSA and BSA through a predominantly static quenching mechanism, with binding constants on the order of 106 M-1. Thermodynamic analysis demonstrated that the binding process is spontaneous and predominantly entropy-driven, with hydrophobic interactions playing a major role in stabilizing the complexes. FRET analysis suggested that HSQ is located in close proximity to the protein fluorophores, with higher energy transfer efficiency observed in the BSA system. Structural analysis using circular dichroism (CD) and FTIR spectroscopy revealed conformational changes in the secondary structure of both proteins upon interaction with HSQ. AFM imaging indicated changes in protein morphology, likely associated with aggregation behavior. Molecular docking results identified the probable binding regions and supported the experimental findings. Overall, this study provides a comprehensive and method-dependent.

T82087

OPTIMIZED MICROWAVE-ASSISTED DISSOLUTION OF COMPLEX GEOLOGICAL AND BATTERY MATRICES FOR ACCURATE TRACE AND SPECIATION ANALYSIS. **Mohammad Reza Gholipour***[1]; Eric Landry [2]. [1] Anton Paar Canada Inc., 2920 Rue de Miniac; [2] Montréal, QC H4S 1N5, Canada. (mohammad.reza@anton-paar.com).

Accurate elemental and speciation analysis in mining, metallurgical, and battery-materials research requires complete dissolution of complex, refractory matrices while preserving analyte integrity. Geological samples—such as chromite ores, REE-bearing rocks, and PGM-rich deposits—and lithium-ion battery components present challenges due to heterogeneous composition, high silicate content, refractory oxides, and carbonaceous phases. This study evaluates high-temperature, high-pressure closed-vessel microwave digestion strategies for these materials. Conditions up to 300 °C and 199 bar enabled efficient decomposition of resistant phases including Al_2O_3-, ZrO_2-, and Cr-rich ores, as well as graphite- and Si/C-based anode materials. Optimized multi-acid systems (HNO_3, HCl, HF or HBF_4, H_3PO_4, H_2SO_4, $HClO_4$) and controlled pressure management minimized losses of volatile and redox-sensitive elements. Certified reference materials for chromium ores, REE-bearing rocks, and PGM-containing matrices showed recoveries consistent with certified values by ICP-OES and ICP-MS, confirming digestion completeness. For battery materials, staged oxidation ensured quantitative decomposition of carbonaceous components, enabling accurate determination of transition metals and trace impurities. Microwave-assisted alkaline leaching of bauxite further demonstrated applicability to process-relevant workflows.These results highlight the effectiveness of optimized microwave digestion protocols in supporting reliable elemental and speciation analysis across resource characterization, metallurgical process control, and advanced energy-materials research.

P750939

ISOLATION OF PRYMNESIN-A2 FROM PRYMNESIUM PARVUM FOR REFERENCE MATERIAL PRODUCTION. **Jack Gillies***[1]; Bruno C. Garrido [1]; Cheryl Rafuse [1]; Ingunn A; Samdal Pearse McCarron[1]; Elizabeth M. Mudge [1]. [1] Metrology Research Centre, National Research Council of Canada, 1411 Oxford Street, Halifax, NS, B3H 3Z1, Canada; [2] Norwegian Veterinary Institute, P.O. Box 64, 1431 Ås, Norway (Jack.Gillies@nrc-cnrc.gc.ca).

Prymnesium parvum is a harmful algal species responsible for significant fish kills worldwide. During blooms, the microalgae produce prymnesins, which are toxic to aquatic organisms. Four prymnesins have been isolated for structural elucidation; however, solubility and stability challenges have hindered reference material availability, leading to poor measurement comparability & reliability for these toxins. To develop a prymnesin reference material, P. parvum UTEX-2797 was cultured in 80-L batches using L1(-Si) medium with a salinity of 10 psu. Following

harvest of the cells and extraction, an isolation procedure using several chromatographic steps was developed for the most abundant A-Type prymnesin analogue PRM A2. The isolation procedure was optimized to balance yield and purity by considering solubility, stability, and recovery. The final purity of PRM-A2 was assessed with LC-UV-CAD-MS and a preliminary feasibility study was completed. Structural confirmation was achieved using 1D- & 2D-NMR spectroscopy, and LC–HRMS. The purified PRM-A2 was quantitated by qNMR, diluted gravimetrically in 9:1 MeOH/DIW (v/v) with 0.1% formic acid, and dispensed as a reference material into argon-purged ampoules. The material was homogenous and demonstrated stability over a 28-day period at various storage conditions. Future efforts will focus on isolating additional prymnesin analogues, and developing methods for environmental monitoring.

T740519

COMBINING MICROFLUIDIC BIOELECTROCHEMISTRY WITH MODELING FOR A DIGITAL TWIN OF ELECTROACTIVE BIOFILMS: VISUALIZING HIDDEN METABOLIC STATES. **Jiao Zhao***; Mir Pouyan Zarabadi; Laurence Yang; Jesse Greener. Département de chimie, Université Laval, 1045 avenue de la médecine, Québec G1V 0A6, Canada. (jesse.greener@chm.ulaval.ca).

Electroactive bacteria exchange electrons with electrodes, powering microbial systems for electricity generation, chemical synthesis, and contaminant remediation. In dense biofilms, metabolism couples tightly to extracellular electron transfer (EET) and mass transport, yet internal organization remains obscured by aggregate electrochemical signals. Here, I present a genome-scale digital twin of a Geobacter sulfurreducens biofilm, combining microfluidic bioelectrochemistry with modeling to visualize hidden metabolic states. The biofilm resides in a microfluidic electrobioreactor, consisting of a 3-electrode device with integrated reference electrode that enables precise chronoamperometry under modulated concentrations and flow rates. Integrating genome-scale metabolic modeling, EET physics, and 3D reactive transport, the model is constrained by these analytical microfluidic electrochemistry measurements to map metabolic activity spatially. Simulations reveal structured metabolism: coupled mass transport and EET limitations reorganize fluxes, causing metabolic segregation and altered substrate oxidation stoichiometry. Misalignment of substrate delivery and zones of electron discharge efficiency suppresses electrical output despite nutrient abundance. These findings demonstrate how electrochemical constraints propagate through metabolism to drive emergent biofilm behavior. This digital-twin tool couples to and extends beyond typical analytical measurements, enabling visualization of otherwise hidden metabolic states for predictive design of electroactive systems in energy, remediation, and synthesis.

T831014

SEPARATION-COUPLED MULTIDIMENSIONAL ANALYSIS OF POLYETHYLENE BIODEGRADATION PRODUCTS REVEALS NANOPLASTICS AND SHORT-CHAIN OLIGOMERS FROM GUT-MICROBE-MEDIATED TRANSFORMATION. **Jesse Greener***; Saqib Ali; Nan Jia; Sabhjeet Kaur;

George C. diCenzo. Département de chimie, Université Laval, 1045 avenue de la médecine, Québec G1V 0A6, Canada (jesse.greener@chm.ulaval.ca).

Polyethylene (PE) is pervasive and is among the most resilient polymers because of its all-carbon backbone, rendering it highly persistent in the environment. Most PE biodegradation studies focus on the remaining plastic film; however, at best these studies provide only indirect evidence of true chemical breakdown and cannot distinguish fragmentation from depolymerization or related chemical modification. The mechanisms of degradation and the fate of the resulting breakdown products remain largely unknown. Here we couple classical film-centric measurements with a new effluent-based analytical strategy centered on chemical separations to resolve hydrophobic breakdown products in complex microbial matrices. After isolation, multi-technique analysis is conducted. FTIR and NMR demonstrate unambiguous oxidation and biodegradation via chain cleavage into oligomers with 8–14 repeat units, while nanoparticle tracking analysis (NTA) and energy-dispersive X-ray spectroscopy (EDX) confirm fragmentation into colloidal nanoplastics. Complementarity between film and effluent analyses shows that materials leaving strong C=O signals on the remaining film yield weaker carbonyl signatures in the oligomers, and vice versa. These results indicate that gut-microbe-mediated PE degradation proceeds beyond simple fragmentation toward partial depolymerization, and underscore the central role of separations-coupled spectroscopic and mass-spectrometric analysis in mapping polymer breakdown mechanisms and product fate in biological systems.

T92018

ENHANCED SENSITIVITY AND QUANTITATIVE PERFORMANCE OF THE SCIEX TRIPLE QUAD 7500+ AND ZENOTOF 8600 SYSTEMS ADDRESS THE CURRENT CHALLENGES IN BIOANALYSIS. **Mahbod Hajivandi***; Mathew Stone [1]; Lakshmanan Deenadayalan [2]; Sashank Pillai [2]; Eshani Galermo [1]; Ebru Selen [1]; Rahul Baghla. [1] SCIEX, India; [2] SCIEX, USA. (mahbod.Hajivandi@sciex.com).

Next generation therapeutics are designed with enhanced potency as well as complexity to increase specificity to their intended target. This presents challenges for bioanalysis where analytical techniques need to evolve to be more sensitive to measure lower doses and more specific to characterize increasingly sophisticatedly designed drugs. Here we will share data from two case studies to showcase the use of ultrasensitive mass spectrometers. The first study describes quantitation of empagliflozin, a compound used for treatment of diabetes mellitus, from dried blood spots using the Triple Quad 7500+ system. A 1 ng/mL LLOQ with an on-column amount of 0.12 pg was achieved demonstrating excellent sensitivity with this assay using microsampling. The second example shows peptide quantification from plasma using the ZenoTOF 8600 system. By summation of fragment ions from an MRMHR experiment LLOQs from 11 to 366 amol on column were achieved. Overall, the sensitivity, linear dynamic range, and reproducibility achieved using these mass spectrometers show that they can address the challenges presented in current bioanalytical assays.

T840617

USING COPPER NANOSPECIES TO ADVANCE CHEMICAL FEEDSTOCK SYNTHESIS: A LIGHT-MEDIATED APPROACH TO SUSTAINABLE PROCESSES. **Geniece L. Hallett-Tapley***; Leah Baylis; Anna Mulak; Lauren Gatto; Jillian Fougere. St. Francis Xavier University, Department of Chemistry, 5009 Chapel Square, Antigonish, NS B2G 2W5, Canada (ghallett@stfx.ca).

Copper nanoparticles are widely regarded as cost-effective alternatives to noble metal nanocatalysts such as gold, silver, platinum, and palladium. In many oxidative and reductive transformations, cuprous oxide (Cu_2O) species are identified as the primary active components. Despite these advantages, large-scale implementation has been hindered by the pronounced oxidative sensitivity of Cu_2O, which leads to reduced catalytic lifetimes and limited recyclability. Such limitations are particularly problematic in industrial contexts, where long-term catalyst reuse is considered a high priority concern. Our research has focused on overcoming this critical barrier, by developing a series of light-activated cuprous oxide nanocomposites. Here, synergetic interactions with metal oxide or carbonaceous supports have proved beneficial for improved catalytic longevity, affording slower rates of Cu+ oxidation and improve reuse. The current contribution will discuss the structural characterisation of these robust Cu2O nanomaterials, followed by their wide-reaching application in clean energy advances and critical chemical feedstock pathways, including nitroaromatic reductions, phenol production, and C-C bond formation. Finally, preliminary work focused on improving the durability of copper-based catalysts will highlight the versatility of visible light-mediated methods as a rapid and effective regenerative tool for extending overall catalyst recyclability.

T940118

NEW INSIGHTS INTO MICROBIAL CARBON CYCLING VIA MARINE METABOLOMICS. **Kathryn H. Halloran***; Brianna Garcia; Natalie Graham; Melissa Kido Soule; Elizabeth B. Kujawinski; Erin M. Bertrand. Department of Biology, Dalhousie University, Halifax, NS, B3H 4R2, Canada (khalloran@dal.ca).

Metabolites dissolved in seawater are important components of the global carbon cycle and mediators of interactions between marine microbes, structuring microbial ecosystems. While important, many dissolved metabolites are exceptionally challenging to measure: they are present in pM to nM concentrations within a mM salt matrix, and their polarity often limits their extraction and chromatographic separation. To address these challenges, we developed a method for measuring dissolved metabolites via pre-extraction aniline derivatization, solid-phase extraction, and liquid chromatography-tandem mass spectrometry (LC-MS/MS). In addition to improved extraction and chromatographic separation, aniline derivatization with isotopically labeled aniline can generate a full suite of stable isotope labeled internal standards, improving quantification. With this method, we can currently measure 51 metabolites with pM to nM limits of detection, 24 of which were not previously analytically accessible. Furthermore, we verify the utility of this method by applying it to

samples from cultures of marine phytoplankton and environmental samples from the southeastern tropical Pacific Ocean.

T940716

EXPLORING THE STRUCTURAL DYNAMICS OF THE BACTERIAL PERIPLASMIC PROTEASE-CHAPERONE DEGP USING METHYL TROSY NMR. **Robert W. Harkness***. University of Guelph Department of Molecular and Cellular Biology. (rharknes@uoguelph.ca).

The DegP protease-chaperone operates within the periplasm of Gram-negative bacteria where it regulates protein homeostasis, promotes virulence, and is essential to survival under stress. DegP forms cage-like complexes which expand to encapsulate substrate proteins of various sizes. Here, we probe DegP cage assembly and host–guest interactions within a 600 kDa DegP cage complex. We leverage a combination of hydrodynamics measurements, methyl TROSY NMR studies, and proteolytic activity assays to map this in detail. Methyl TROSY data indicate that DegP forms a network of preorganized apo oligomers that facilitates the capture of substrates within cage distributions. We find that in the presence of a model client, DegP cages assemble cooperatively with few intermediates. Our data further show that the N-terminal half of the bound client, which projects into the interior of the cages, is predominantly unfolded and flexible, exchanging between multiple conformational states over a range of time scales. Finally, we reveal that a concerted structural transition of the protease domains of DegP occurs upon client engagement, leading to activation. Together, our findings support a model of DegP as a highly cooperative and dynamic molecular machine that stabilizes unfolded states of clients, giving rise to eXicient proteolysis.

T740517

EFFECT OF SURFACE OXIDATION ON SIMULATED SURFACE-ENHANCED RAMAN SPECTROSCOPY WITH SILVER NANOPARTICLES. **Scott G. Harroun***. Department of Chemistry and Biochemistry, University of Windsor, Windsor, Ontario, Canada (scott.harroun@uwindsor.ca).

Surface-enhanced Raman spectroscopy (SERS) is the enormous boost in Raman signal intensity when a molecule is on or near the surface of plasmonic nanomaterials, such as gold or silver nanoparticles. Beyond analytical detection, SERS can also be used to probe the orientation of molecules adsorbed on nanoparticle surfaces. This is often achieved by employing density functional theory (DFT) to simulate spectra for a molecule of interest interacting with a model surface in a variety of orientations. The simulated spectrum displaying the best agreement with the experimental spectrum indicates the likely adsorption orientation. The model surface is typically an atom, ion, or cluster. For silver, classic model surfaces include Ag, Ag+, Ag4 and Ag4+. However, these neglect the presence of silver oxide that often forms on silver nanoparticles when exposed to atmospheric oxygen. This talk will demonstrate that using Ag2O as a model surface can provide simulated spectra that more closely reproduce experimental SERS data.

T91092

MEASUREMENT OF TRACE LEVELS OF ANATOXINS IN NOVA SCOTIA FRESHWATER SYSTEMS USING LC-MS/MS AND DART-HRMS/MS. **Sophie Haverstock***[1,2]; Rob C. Jamieson [1]; Daniel G. Beach [1,2]. [1] Department of Civil & Resource Engineering, Dalhousie University, Halifax, NS, Canada; [2] Metrology Research Center, National Research Council of Canada, Halifax, NS, Canada (Sophie.Haverstock@dal.ca).

Canine deaths have been reported globally following the ingestion of Microcoleus cyanobacterial mats containing anatoxins, a potent class of neurotoxins. Anatoxin concentrations in benthic mats have been well studied, however, little is known about concentrations in overlying waters due to low toxin levels. Microcoleus mats have been found in freshwater used for drinking water and recreation, highlighting the need to improve low-level anatoxin detection in water. To achieve this, two methods were developed including increasing LC-MS/MS injection volumes which reduced the homoanatoxin LOD to 0.02 µg/L, and incorporating an offline SPE preconcentration prior to LC-MS/MS analysis which reduced the homoanatoxin LOD to 0.004 µg/L. Ongoing work is evaluating pipette tip SPE coupled to DART-HRMS/MS for rapid detection. To test these methods, two interconnected urban lakes in Dartmouth, Nova Scotia, were sampled weekly from May to July 2025, collecting mat and overlying water samples. Homoanatoxin was the most abundant anatoxin in mat and water samples, and all anatoxin concentrations were below the World Health Organization recreational limit of 60 µg/L, however, impacts of chronic low-level anatoxin exposure remain unclear, emphasizing the importance of increased sensitivity. Together, these methods improve low-level anatoxin detection in water and provide flexible analytical options.

T930713

INVESTIGATING THE SOLUTION STABILITY OF A HYDROPHOBIN FROM SCHIZOPHYLLUM COMMUNE. **Raymond He***. Department of Chemistry, Dalhousie University, Chemistry Building, 6274 Coburg Road, Halifax, NS B3H 4R2, Canada (Raymond.He@dal.ca).

Hydrophobins are small secreted proteins that play vital roles in the growth and development of filamentous fungi. They can also self-assemble into larger structures called rodlets that coat surfaces such as fungal spores, making them extremely water repellent. Hydrophobins can be used to modify surfaces to prevent fouling or biofilm formation, as new drug delivery agents, as biosensors, and to make hydrophobic surfaces more biocompatible, which is important for the success of medical implants. It is necessary to understand the structure and self-assembly mechanisms of hydrophobins so that their properties can be controlled and applied. This project focuses on SC16, a model hydrophobin from Schizophyllum commune. Since hydrophobins undergo a structural transition when interacting with a surface the to form rodlets, studying the stability of SC16 in solution may indicate which regions of the protein are most amenable to structural changes at a surface. Thus, SC16 stability against heat, chemical denaturation, and

reducing agents were monitored using 1H-15N heteronuclear single quantum coherence nuclear magnetic resonance. SC16 is extremely stable and shows high resistance to heat denaturation. Additionally, 8M urea does not denature SC16 and chemical shift perturbations appear to be due to solvent effects on the protein instead of larger unfolding processes. Finally, the reducing agent dithiothreitol reduces disulfide bonds of SC16 but leaves its tertiary structure intact. Overall, this work highlights the extraordinary resistance of SC16 to heat and denaturation, even before assembly into rodlets at a surface.

T830615

POINT OF CARE DIAGNOSIS OF VITAMIN D. **Onur Bulut***; Kevin Hewitt. Dalhousie University, Department of Physics and Atmospheric Science, 6310 Coburg Road, Halifax, NS B3H 4R2, Canada (kevin.hewitt@dal.ca).

Vitamin D deficiency is associated with osteoporosis, immune dysfunction, and is more prevalent in Black populations. Emerging evidence also indicates a relationship between vitamin D deficiency and the development and progression of uterine fibroids. Reliable detection of 25-hydroxyvitamin D3 (25-OH-D3), the primary serum marker of vitamin D status, remains challenging due to its low concentration and the need for complex analytical instrumentation. Here, we present a label-free colorimetric biosensor based on gold nanoparticles (AuNPs) functionalized with a vitamin D binding aptamer (VDBA14) for the rapid detection of 25-OH-D3 [2]. A complementary probe sequence, separately conjugated to AuNPs, induces nanoparticle aggregation through aptamer-probe hybridization in the absence of the target. When 25-OH-D3 is present, aptamer binding prevents hybridization, preserving colloidal stability and producing a visible color difference. Preliminary results confirm sequence-specific aggregation and the feasibility of this competitive mechanism. Ongoing studies evaluate the sensitivity and selectivity of the system using spectroscopic measurements. This platform offers a simple, cost-effective approach for vitamin D detection with potential applications in clinical diagnostics and point-of-care testing.

T730413

QUANTIFYING LEAD IN TATTOO INKS. **Adelaide Treibley***; Alison Holliday. Moravian University, Department of Chemistry, 1200 Main Street, Bethlehem, PA, 18018, USA (hollidaya@moravian.edu).

Acid digestion followed by Graphite Furnace Atomic Absorption Spectrometry was used to quantify lead in tattoo inks of various colors from the same manufacturer. Lead concentration varied considerably by color, with results ranging from 30 ppb to 1.4 ppm. Most inks had average lead concentrations above the suggested safe limit of 70 ppb [1]. There was also large variation in lead concentrations between samples from the same bottle, suggesting uneven suspension of lead-containing particles in the ink.

T81023

RAPID DISCOVERY-TO-SCREENING OF BACTERIOPHAGES USING A COLORIMETRIC ASSAY AND AI-BASED ANALYSIS SYSTEM. **Ekaterina Kvitka***[1]; Akansha Prasad [2]; Saakshi Arvikar [3]; Carlos D. M. Filipe [1]; TohidF Didarb [4,5]; Zeinab Hosseinidoust [1,2,5,6]. [1] Department of Chemical Engineering, McMaster University, Hamilton, Ontario, L9S 8L7, Canada; [2] School of Biomedical Engineering, McMaster University, Hamilton, Ontario, L9S 8L7, Canada; [3] School of Interdisciplinary Science, McMaster University, Hamilton, ON L8S 4L7, Canada; [4] Department of Mechanical Engineering, McMaster University, Hamilton, Ontario, L9S 8L7, Canada; [5] Michael DeGroote Institute for Infectious Disease Research, McMaster University, Hamilton, Ontario, L98 4L8, Canada; [6] Farncombe Family Digestive Health Research Institute, McMaster University, Hamilton, Ontario, L8S 4K1, Canada (doust@mcmaster.ca).

Antimicrobial resistance (AMR) continues to accelerate globally, increasing the burden of hard-to-treat infections across clinical and agricultural settings. Bacteriophage (phage) therapy offers a targeted alternative to antibiotics, but its practical deployment depends on rapid discovery and matching of effective phages against relevant bacterial strains, particularly patient-derived clinical isolates. Conventional workflows for phage hunting and screening are often slow, labor-intensive, and dependent on specialized infrastructure, limiting responsiveness when time-to-treatment is critical. To address this bottleneck, we developed a rapid, scalable phage discovery-to-screening pipeline that combines environmental phage sourcing with fast colorimetric testing and AI-enabled interpretation. Methods. Environmental samples, with an emphasis on wastewater, were collected as high-diversity reservoirs for isolating phages active against clinical bacterial isolates. Following enrichment and purification, candidate phages were screened using a colorimetric assay that reports phage-induced bacterial lysis through a visible and quantifiable signal change. Assay outputs were analyzed using an AI-driven classification model capable of assigning either a two-class outcome (active/inactive) or a three-class outcome (low/moderate/high activity), enabling flexible deployment depending on the use case. To support field-forward and high-throughput operation, the two-class model was optimized for smartphone imaging, while the three-class model was paired with an automated imaging setup for enhanced quantitative consistency. Lead phage candidates were further characterized using transmission electron microscopy (TEM) for morphology, and genomic sequencing was initiated to support phage identification, safety profiling, and library development. In parallel, the screening platform was stabilized using a sugar–polymer matrix to enable a shelf-stable, commercially relevant 96-well plate format. Results and conclusion. The platform enabled functional phage screening and activity classification in under 3 hours, representing a substantial acceleration compared with conventional workflows requiring overnight growth and manual interpretation. AI-assisted analysis achieved high classification performance in both simplified (two-class) and granular (three-class) outputs, improving reproducibility while reducing reliance on specialized equipment. Importantly, integrating wastewater-derived sampling directly into the workflow enabled rapid identification of candidate phages active against clinical

isolates, accelerating early-stage discovery and narrowing the search space for downstream therapeutic development. TEM confirmed diverse phage morphologies among lead candidates, and sequencing is underway to establish genomic identity and inform future formulation and translational work. Collectively, this work positions the platform as a scalable solution for fast phage discovery and matching, enabling more responsive phage therapy development across clinical and applied settings.

T731011

SORTING CHIP ONLINE COUPLED WITH ICP-MS FOR CIRCULATING TUMOR CELLS DETECTION. **Bin Hu***. Wuhan University, Department of Chemistry, Wuhan, China 430072 (binhu@whu.edu.cn).

The detection of circulating tumor cells (CTCs) provides valuable clinical information for cancer diagnosis and monitoring. However, the rarity and high heterogeneity of CTCs, along with the complexity of blood samples, pose significant challenges for their isolation and accurate detection from blood. Inductively coupled plasma mass spectrometry (ICP-MS), as a powerful elemental analysis technique, can provide quantification of target cells and assess specific protein expression levels via exogenous elemental tags. Microfluidic sorting chips enable precise control of cell displacement and high-throughput cell analysis. In this presentation, the potential of cascaded sorting chips combined with elemental labeling ICP-MS for CTCs detection will be illustrated [1-5]. This approach offers an efficient alternative to traditional CTCs detection methods, enabling specific and high-through detection of CTCs in actual clinical blood samples.

T930711

A NEW NMR PROTOCOL FOR DETERMINING PROTEIN SIDE CHAIN ROTAMERS USING 1H RELAXATION AND J COUPLINGS. **Peter M. Hwang***[1]; David Case [2]. [1] Departments of Medicine and Biochemistry, 3-08 Medical Sciences Building, University of Alberta, Edmonton, Alberta, Canada T6G 2H7 ; [2] Department of Chemistry and Chemical Biology, Rutgers University (phwang1@ualberta.ca).

Many side chains in folded protein domains are mobile, able to access multiple side chain rotamers (gauche+, gauche-, or trans) via large 120º jumps. Which side chains are mobile is not always clear from conventional structures determined by crystallography, cryo-EM, or NMR. We propose that initial 1H relaxation rates are reliable indicators of side chain mobility, most easily accessible by appending a 1H-TOCSY element to the beginning of any multidimensional NMR experiment beginning on 1H Selecting the correct side chain motional model is essential for proper interpretation of side chain NMR J couplings, which reflect a weighted average of rotamer populations. Usage of empirically derived Karplus coefficients (describing the relationship between side chain dihedral angle and J couplings) yielded spurious side chain conformations not consistent

with molecular dynamics simulations. This inconsistency was resolved using de novo Karplus coefficients derived with density functional theory (DFT). We speculate that the Karplus coefficients most widely used by the NMR community were inaccurate because they were derived using limited data that included mobile residues. Our new methodology allows for precise determination of average dihedral angles +/- 1-2 degrees for rigid side chains, as well as reasonable estimates of rotamer populations for mobile residues.

T730511

AN ELECTROCHEMICAL MONITORING OF THROMBIN ACTIVITY USING AN ELECTROGENIC SUBSTRATE. **Anna Ignaszak***; Sina Ardalan. Brock University, Department of Chemistry, 1812 Sir Isaac Brock Way, St. Catharines, ON L2S 3A1, Canada. (aignaszak@brocku.ca).

Monitoring blood coagulation is critical for assessing bleeding and cardiac disorders. A variety of bioanalytical techniques for coagulation analysis are based on measuring the activity of a key enzyme, thrombin. Recent advances in electrochemical analyzers have enabled miniaturized systems for rapid thrombin activity analysis, but a key challenge is the lack of universally available electrogenic substrates. This work presents a proof-of-concept electrochemical biosensor for continuous thrombin monitoring using a widely available peptide-based substrate. The measuring system consists of a screen-printed gold electrode and the substrate, Phe-Pip-Arg para-nitroanilide, which is cleaved by thrombin to liberate para-nitroaniline (pNA). We developed a square wave voltammetry technique to measure the oxidation current of the liberated pNA in just seconds, with a total sample volume of only 100 µL and a detection limit of 0.24 nM. The developed assay is compatible with self-assembled monolayer-functionalized electrodes, which are highly demanded in biosensor research, such as aptamer-based sensors. We found that thrombin retains its activity on gold and even on anti-biofouled electrodes treated with mercaptohexanol. Our enzymatic amplification method can be integrated into coagulation analyzers and thrombin generation assays, while providing a better understanding of protein activity and biofouling on self-assembled monolayers.

T830211

A PLASMA-ENHANCED FABRICATION AND REGENERATION OF A BIOSENSOR PLATFORM. **Anna Ignaszak***[1]; Sina Ardalan [1]; Clara Tran [2]; Stuart T. Fraser [2]; Marcela Bilek [2]. [1] Brock University, Department of Chemistry, 1812 Sir Isaac Brock Way, St. Catharines, ON L2S 3A1, Canada; [2] School of Biomedical Engineering, J03, The University of Sydney, NSW 2008, Australia, Culturon Pty Ltd, School of Physics, A28, The University of Sydney, NSW 2006, Australia. (aignaszak@brocku.ca).

Miniaturized electroanalytical devices with screen-printed electrodes (SPE) are popular for their compact size and low analyte requirements. However, their single-use nature and non-degradable polymer substrates with printed precious metals like gold limit sustainability. Disposing of each electrode after use is costly and unsustainable. Here, a green air plasma cleaning technique regenerates multiple gold SPEs simultaneously. A 1.2-fold increase in electroactive surface area led to a 2-fold increase in aptamer immobilization and a 3-fold enhancement in sensor signal. Air plasma cleaning is a sustainable, simple method to regenerate gold SPEs, enhancing probe loading and biosensing sensitivity [1]. A key step in creating a heterogeneous biosensor is immobilizing the biorecognition element on the sensing substrate. Typically, this involves self-assembled monolayers of thiol-modified capture probes on metals, or chemical reactions such as carbodiimide bioconjugation, glutaraldehyde crosslinking, or click chemistry. These methods all require multi-step wet chemical reactions. In this study, we used plasma-activated coating (PAC), a plasma-enhanced chemical vapour deposition method, to directly attach a DNA-based aptamer onto a screen printed carbon electrode. The PAC surface contains radicals that covalently link linker-free DNA aptamers without the use of chemical agents. PAC modification allows high-density aptamer immobilization without wet chemistry, enabling a biosensing platform. [1] Sina Ardalan, Clara T. H. Tran, Stuart T. Fraser, Marcela Bilek, Anna Ignaszak, RSC Sustainability, 2026, Under review.

T82018

ANALYTICAL STRATEGIES IN THE PROFILING OF BREATH VOLATILES: APPLICATION OF HEADSPACE SOLID-PHASE MICROEXTRACTION. **Zhehan Jiang***[1]; Laura Elliott [2]; Sarah DeGrace [2]; Simon Gadbois [2]; Sherry H. Stewart [2]; Suzanne M. Budge [1]. [1] Dalhousie University, Department of Process Engineering and Applied Science, 5273 DaCosta Row, Halifax, NS; [2] Dalhousie University, Department of Psychology & Neuroscience, 6287 Alumni Crescent, Halifax, NS (zh417721@dal.ca).

The remarkable ability of canine olfaction to detect disease-specific odors provides compelling evidence of the rich diagnostic information contained within human exhaled breath; however, the specific volatile organic compounds (VOCs) and chemical compositions perceived during these biological responses remain poorly defined. Detecting these trace-level biomarkers requires exceptional analytical sensitivity and selectivity. To address these hurdles in our ongoing research, we have adopted the Markes' BioVOC-2™ as a standardized breath sampler, while utilizing headspace solid-phase microextraction coupled with gas chromatography-mass spectrometry to overcome the complex challenge of trace-level pre-concentration. We investigated differences in VOCs from individuals with trauma histories (66% with post-traumatic stress disorder) and compared breath samples taken during exposure to personalized trauma or neutral cues, utilizing baseline breath collected before each cue exposure as a control. Although isolating true biological markers within the massive datasets generated by untargeted profiling remains a long-term goal, more than 50 VOCs, including aldehydes such as hexanal, octanal and nonanal which are related to lipid metabolism, were successfully detected across 20 participants' samples tested thus far. Preliminary

principal component analysis of the total volatile profiles demonstrated distinct clustering between neutral and trauma samples.

T82016

ARE WE BREATHING IN SIDECHAIN FLUOROPOLYMER MICROPLASTICS? INSIGHTS FROM ION MOBILITY MASS SPECTROMETRY. **K.J. Jobst***[1]; J.R. Bissonnette; G.C. Lastoria; M. Aghaei; N. Harvey; E.C. Tolefe; M.L. Rowsell; S. Brandsma [2]. [1] Department of Chemistry, Memorial University of Newfoundland, St. John's, NL, Canada; [2] A-LIFE Labs, Vrije Universiteit Amsterdam, Amsterdam, The Netherlands (kjobst@mun.ca).

Per- and polyfluoroalkyl substances are often applied as a topical treatment to improve a material's water/oil repellency [1], but their effectiveness declines with wear. Consequently, polymeric textiles, including fibers, yarns, carpets, and garments, have been functionalized with covalent-bound perfluoroalkyl chains, viz. sidechain PFAS, to improve durability. While concerns over drinking water exposure are well known, humans may also be exposed to PFAS by inhalation of sidechain fluoropolymer microplastics [2] shed from textiles, consumer products and coatings that become suspended in indoor air. Inspired by Skedung et al. [3], we developed a novel method that couples pyrolysis gas chromatography with ion mobility mass spectrometry, enabling simultaneous characterization of microplastics and plastics additives, including PFAS.When applied to indoor air particulate, indoor dust, and water repellent fabrics collected from St. John's, the method revealed: (i) the concentration of polymer bound PFAS could greatly exceed free PFAS; and (ii) the presence of previously undocumented PFAS potentially originate from waterproof polymers. These results underline the need to better understand exposure to sidechain fluoropolymer microplastics.

P750120

THE CIRCULATING LIPIDOME ASSOCIATES WITH WHITE MATTER DAMAGE IN VASCULAR COGNITIVE IMPAIRMENT (VCI) AND IMMUNOGLOBULIN G INDEX IN MULTIPLE SCLEROSIS. **Zahra Kanaan***[1,2]; Thao Nguyen-Tran [1]; Miroslava Cuperlovic-Culf [3]; Eric Smith [4]; Guila Fadda [2]; Steffany AL Bennett [1,2]. [1] Neurolipidomics Lab, India Taylor Lipidomic Research Platform, Ottawa Institute of Systems Biology, Department of Chemistry and Biomolecular Sciences and Department of Biochemistry, Microbiology and Immunology, University of Ottawa; [2] Neuroscience, Ottawa Hospital Research Institute, The Ottawa Hospital and Department of Cellular and Molecular Medicine, University of Ottawa; [3] Digital Technologies Research Centre, National Research Council of Canada, Canada, Ottawa, ON; [4] Department of Clinical Neurosciences, University of Calgary, Calgary, Alberta, Canada. (zkanaan@uottawa.ca).

Aberrant lipid metabolism is associated with vascular cognitive impairment (VCI) and multiple sclerosis (MS). VCI is a cerebral small vessel disease (cSVD) accounting for approximately 30% of all

dementia cases. cSVD is defined in magnetic resonance imaging (MRI) by small subcortical infarcts, lacunes, and white matter hyperintensities (WMHs). MS is an autoimmune and demyelinating disorder of the central nervous system also defined by WMH. Whether lipid changes are specific to VCI-associated WMHs or reflect the presence and extent of neuroinflammation in other disorders, such as MS, remains unclear. To explore this question, we have profiled the circulating lipidome in a discovery cohort of cognitively normal controls, in persons with VCI, and in persons with MS. We used nanobore liquid chromatography-electrospray ionization-tandem mass spectrometry (nLC-ESI-MS/MS) in multiple-reaction-monitoring (MRM) mode for quantification verifying structures using independent data acquisition, enhanced product ion (IDA-EPI) scan. We show that changes in the circulating levels of Cer(d18:1/19:0), Cer(d18:1/20:0), Cer(d18:1/21:0), Cer(d18:1/22:0), Cer(d18:1/23:0) associate with both VCI and MS. In VCI, these levels associate with WMH volume. In MS, the ceramide lipidome associates with the IgG index These data provide preliminary evidence to suggest that the circulating sphingolipidome may serve as a useful correlate of neuroinflammation and WMH.

T930714

MAPPING THE MOLECULAR FEATURES AND FUNCTIONAL ROLES OF INTRINSICALLY DISORDERED REGIONS IN KATP CHANNELS. **Voula Kanelis***. Department of Chemical and Physical Sciences, University of Toronto Mississauga; Departments of Chemistry, and Cell and Systems Biology, University of Toronto (voula.kanelis@utoronto.ca).

Hydrophobins are small secreted proteins that play vital roles in the growth and development of filamentous fungi. They can also self-assemble into larger structures called rodlets that coat surfaces such as fungal spores, making them extremely water repellent. Hydrophobins can be used to modify surfaces to prevent fouling or biofilm formation, as new drug delivery agents, as biosensors, and to make hydrophobic surfaces more biocompatible, which is important for the success of medical implants. It is necessary to understand the structure and self-assembly mechanisms of hydrophobins so that their properties can be controlled and applied. This project focuses on SC16, a model hydrophobin from Schizophyllum commune. Since hydrophobins undergo a structural transition when interacting with a surface the to form rodlets, studying the stability of SC16 in solution may indicate which regions of the protein are most amenable to structural changes at a surface. Thus, SC16 stability against heat, chemical denaturation, and reducing agents were monitored using 1H-15N heteronuclear single quantum coherence nuclear magnetic resonance. SC16 is extremely stable and shows high resistance to heat denaturation. Additionally, 8M urea does not denature SC16 and chemical shift perturbations appear to be due to solvent effects on the protein instead of larger unfolding processes. Finally, the reducing agent dithiothreitol reduces disulfide bonds of SC16 but leaves its tertiary structure intact. Overall, this work highlights the extraordinary resistance of SC16 to heat and denaturation, even before assembly into rodlets at a surface.

P750124

INVESTIGATING THE IMPACT OF SDS ON LC - MS DETECTION OF TRACE LEVEL PROTEINS. **Coumba Habi Kanoute***; Alan A. Doucette. Department of Chemistry, Dalhousie University, Halifax, NS B3H 4R2, Canada (c.kanoute@dal.ca).

The analysis of proteins by LC–MS is highly sensitive to contaminants such as sodium dodecyl sulfate (SDS) which is widely used in bottom-up proteomics. Previous work has established that SDS can be tolerated up to approximately 0.01% without significant loss of signal [1]; however, it remains unclear whether this threshold is maintained at trace-level protein concentrations, where ion suppression effects may be amplified. In this study, the impact of SDS on signal performance was investigated using lysozyme at low concentration. Samples containing varying concentrations of SDS were analyzed by LC–MS to evaluate changes in signal intensity, peak quality, and detection efficiency. Attention was given to assessing whether the established SDS tolerance threshold remains applicable under trace-level conditions. The results indicate that ion suppression effects are more pronounced at lower protein concentrations, suggesting that effective SDS tolerance depends on the protein-to-SDS ratio rather than a fixed threshold. This work highlights the need for optimized sample preparation for reliable detection of low-abundance proteins.

T830711

THE ESSENTIALITY OF SOLUTION NMR SPECTROSCOPY IN THE POST-ALPHAFOLD ERA. **Lewis Kay***. Department of Chemistry, Lash Miller Chemical Laboratories, 80 St. George Street Toronto, ON M5S 3H6, Canada (lewis.kay@utoronto.ca).

Protein dynamics are critical for function and many of nature's molecules are highly dynamic. In this talk I will describe applications to several important systems that are now possible using new solution NMR approaches, including studies of molecular machines, of phase separation at atomic resolution, and of sparsely populated and transiently formed protein conformers that are invisible to most of the techniques of structural biology.

T840216

DESIGNING NEW APPROACH METHODS AND ANALYTICAL TECHNIQUES TO EVALUATE CELL-BASED IMMUNOTHERAPEUTICS. **Joseph Kinsella***. Department of Bioengineering, McGill University (joseph.kinsella@mcgill.ca).

Evaluating cellular immunotherapy in physiologically relevant human tumor models remains a fundamental challenge in preclinical research. Conventional animal models inadequately capture

human tumor-immune dynamics, as such New Approach Methods (NAMs) have been proposed that integrate patient-derived biological complexity with quantitative analytical precision and engineering reproducibility. In this talk we present bioprinted NAMs as potential preclinical models to evaluate cell-based immunotherapy efficacy, activity, and exhaustion. To do this we have developed models that spatially organize patient-derived tumor organoids (PDOs) and autologous tumor-infiltrating lymphocytes (TILs) within a mechanically tunable extracellular matrix hydrogel. This enables longitudinal, multiplexed quantification of immune cell migration, degranulation, and cytokine secretion within a physically defined 3D microenvironment. Orthogonal analytical readouts including confocal microscopy, flow cytometry, and Luminex based multiplex cytokine profiling allow us to measure spatiotemporal TIL dynamics. Critically, TIL migratory data can be integrated into a deterministic reaction-advection-diffusion mathematical model. Together, these methods constitute a modular, patient-specific NAM that bridges biomaterial engineering, quantitative imaging, and computational modeling to functionally characterize immune effector fitness and preclinical evaluation of adoptive cell therapies in solid tumor like microenvironments.

T730415

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

The Yellowknife Garden Metal Study (YKGMS) was initiated to address concerns about the impact of legacy mining in the area in light of the increase of agricultural initiatives in Yellowknife and increasing popularity of growing vegetables for personal consumption. The study was designed to quantify and understand the impacts of potentially harmful elements resulting from the historical mining activities. Arsenic concentrations in garden vegetables were found to be higher than concentrations published by Health Canada in vegetables from grocery stores, although most garden soil concentrations were within concentration ranges typical of background in the area. Concentrations were lower than those measured 20 years earlier. In contrast, the concentrations of selected nutritional elements (calcium, potassium, iron, and zinc) in Yellowknife vegetables were higher than those found in grocery store vegetables. The arsenic concentrations in vegetable and soil concentrations have been contextualized in a human health risk assessment, which was presented to the community in February 2026.

T81082

THE CURIOUS CORRELATION BETWEEN MERCURY AND ARSENIC IN MUSHROOMS. **Iris Koch***. Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 12 Verité Ave, 17000 Station Forces, Kingston, ON K7K 7B4, Canada (koch-i@rmc.ca).

Arsenic and mercury are known to accumulate in some kinds of mushrooms, including edible species, and the toxicity of these two elements has driven some of the past research in this area. Our research group has conducted comprehensive studies on arsenic speciation in mushrooms [1], showing the predominance of non-toxic arsenobetaine in some edible (as well as poisonous) mushrooms (e.g., puffballs). Investigations into the formation of arsenobetaine led to theories about the potential function that arsenobetaine may have in some species [e.g., 2,3]. The enrichment of mercury in puffballs identified in a study of mushrooms collected from Iqaluit [4] led to a survey of mercury concentrations in archived mushroom samples for which arsenic speciation has been determined [1,3]. A correlation between mercury and arsenobetaine concentrations in mushrooms was identified, and the presentation will include a review of the literature to propose hypotheses or future avenues of work to determine the reasons for this correlation.

T82096

CHARACTERIZATION OF PER- AND POLYFLUORINATED ALKYLATED SUBSTANCES (PFAS) IN AQUEOUS FILM-FORMING FOAMS (AFFF) FOR FIREFIGHTING IN SOURCES, FIREFIGHTING VEHICLES, AND THE ENVIRONMENT. **Iris Koch***; Adrian Pang; Chris Kocur; Dean Morrow; Taylor Vereecken; Kela Weber. Royal Military College of Canada, Department of Chemistry and Chemical Engineering, 12 Verité Ave, 17000 Station Forces, Kingston, ON K7K 7B4, Canada (koch-i@rmc.ca).

Per- and polyfluorinated alkylated substances (PFAS) are a large class of toxic and persistent chemicals that were historically added to aqueous film-forming foams (AFFF) that are used to fight fuel fires, and these foams have been used in aircraft rescue and firefighting vehicles (ARFFVs) for decades. The PFAS compounds found in more than 10 AFFFs will be summarized, along with those found in ARFFVs. Linkages between these compounds at a known spill site and findings of PFAS in the environment at the site will be discussed. The focus will be on PFAS compounds identified through suspect screening using liquid chromatography high resolution mass spectrometry, precursors identifiable through a total oxidizable precursor assay, and total organic fluorine; this is a combined approach that promotes the development of a comprehensive picture of PFAS sources and environmental fate.

T92015

PEPTIDE SEPARATION SELECTIVITY UNIVERSE: A GLOBAL OVERVIEW OF REVERSED-PHASE FULLY POROUS SEPARATION MEDIA FOR BOTTOM-UP PROTEOMICS. **Oleg Krokhin***; Vic Spicer. University

of Manitoba, Department of Internal Medicine University of Manitoba, Winnipeg, Canada (oleg.krokhine@umanitoba.ca).

Reversed-phase peptide chromatography is approaching its 50 anniversary, marked by a significant advancement in stationary phase manufacturing, spanning an array of impactful applications including very powerful proteomic techniques. Fully porous silica based stationary phases lead the application landscape using formic acid as ion-pairing additive in water/acetonitrile gradient settings. There is still a significant gap in understanding peptide separation selectivity in reversed-phase separation: what are the driving factors in varying separation selectivity between different C18 (C8, C4, aromatic ligands) of different pore sizes? To address these questions, we evaluated more than 40 different stationary phases (60-300 Å pore size range, C18, C12, C8, C4, CSH C18, phenyl-hexyl, phenyl, pentafluorophenyl) using a standard proteomics nanoflow LC-MS. We performed LC-MS analyses of a Jurkat whole cell tryptic digest (~500 ng) under nearly identical chromatographic conditions [1] using data-dependent mass-spectrometry (Orbitrap Exploris 480) settings with formic acid or TFA as ion-pairing modifiers. LC-MS analyses resulted in identification on average of ~36 and 48 thousand unique peptides for TFA and FA based eluents, respectively. This presentation will provide the first in-depth exploration of peptide separation selectivity across reversed-phase materials with different ligand chemistries.

T730414

ELEMENTAL ANALYSIS OF FOOD AND DRINKING WATER USING NEXION 1100 ICP-MS SYSTEM.

Sandeep Kumar*; Aaron Hineman. Perkin Elmer Scientific Canada ULC 501 Rowntree Dairy Rd., pWoodbridge, ON, L4L8H1, Canada (sandeep.kumar@perkinelmer.com).

Safe and reliable Food and Drinking Water is growing concern because of pollution and can impact public health. Water and Food sources can be contaminated by natural geological processes or by human activities, including the introduction of metal and metalloid elements. Therefore, it is important that all food and drinking water are monitored for toxic elements such as As, Cd, Hg, and Pb. It is also equally important to monitor macronutrients such as Ca, K, Fe etc. Inductively coupled plasma mass spectrometry (ICP-MS) is an ideal analytical technique for this type of application, offering low detection limits, a wide dynamic range, and multi-element capability. In this work, we will present analytical conditions for determination of metals in variety of food matrices and drinking water utilizing Nexion 1100 ICP-MS system. This work demonstrates the ability of the NexION® 1100 ICP-MS to meet and exceed the requirements of various regulations. We will also present system performance data on Nexion 1100 in terms of detection limits, accuracy, and stability during extended operation

P750938

ENHANCED ELECTROCHEMICAL DETECTION OF PER- AND POLYFLUOROALKYL SUBSTANCES USING SELF ASSEMBLED MONOLAYERS FOR APPLICATION IN SOIL WASHING. **Caroline Kupczyk***. Queen's University, Department of Civil Engineering, Dr. Zhe She, Queen's University, Department of Chemistry; Dr. Xiaying Xin, Queen's University, Department of Civil Engineering

(18ck15@queensu.ca).

Per- and polyfluoroalkyl substances (PFAS) are a class of persistent emerging contaminants that pose health and environmental risks. Although current detection methods are sensitive and robust, high costs, limited availability, and non-portable instrumentation make real-time research difficult. Electrochemical sensing, therefore, presents a promising low cost, portable, and more rapid method to detect these trace contaminants in water. Early results indicate detection using bare gold electrodes can be enhanced kinetically through surface modifications to increase hydrophobicity. This research, therefore, focuses on improving the adsorption kinetics of PFOA and PFOS, two model PFAS compounds, to gold electrodes using Self-assembled Monolayers. Using voltametric techniques will enable quantification of signal suppression to determine PFAS concentrations. For application purposes, interference testing involving organic matter and ions will highlight viability of this technique in real water samples. This sensor development will support advancement of future work through rapid in-lab detection of PFAS contaminated water from soil washing to support the United Nations Sustainable Development Goals, Clean Water and Sanitation and Life on Land.

T740516

ELECTROFYING BIOFILMS - PROBING TRANSPORT AND REACTIVITY BY SCANNING GEL ELECTROCHEMICAL MICROSCOPY. **Sabine Kuss***[1]; M. L. Yusuf [1]; M. Saley1, L. Liu [2]. [1] Department of Chemistry, University of Manitoba, Winnipeg, Canada; [2] CNRS, Université de Lorraine, Nancy, France (sabine.kuss@umanitoba.ca).

Scanning Gel Electrochemical Microscopy (SGECM) employs microelectrodes that contain a flexible gel at the electrode-surface interface.1 In the literature, this technique has been applied to hydrophobic substrates.2–5 However, challenge arises when probing hydrophilic surfaces, as gel electrodes become unstable under such conditions, which limits their application to biological systems severely. This presentation reports the development of strategies to improve gel stability when probing hydrophilic substrates. To this end, the shape of the gel electrode was controlled by optimizing key parameters, including the RG of the microelectrode, gel solution pH, and deposition potential. Stability of the gel when probing hydrophilic substrate was achieved by unifying the solvent composition of the gel electrode and substrate. For the first time, SGECM was successfully conducted on agar substrates, where ferrocenemethanol embedded within the agar gel was detected by SGECM as it diffuses through the gel electrode to the electrode tip. These findings highlight the potential of SGECM for potential future biological applications, particularly in studying

biofilms. Biofilms are important target with hydrophilic surface where gel probes could be used for tracking molecular transport through gel-to-gel interactions.

T91093

TERRESTRIAL DOM DRIVES TRACE METAL TRANSPORT IN AGRICULTURAL WATERSHED. **Mary Chris Lagumen***[1]; Lisa Harris [1]; , Taryn Petrovsky [1]; , Kelly Biagi [2]; Vaughn Mangal [1]. [1] Department of Chemistry, Brock University, St. Catharines, ON; [2] Department of Earth Sciences, Brock University, St. Catharines, ON (uu22sv@brocku.ca).

Trace metal mobility in agricultural watersheds is strongly influenced by dissolved organic matter (DOM), yet the mechanisms controlling these interactions remain poorly constrained. This study investigated the spatiotemporal variability of DOM and its role in trace metal transport from April to October 2023 in an agriculturally impacted watershed in southern Ontario, Canada. Hydrological and stable isotope analyses indicated that streamflow was dominated by shallow soil water inputs (70–90%), emphasizing the importance of near-surface flow pathways in mobilizing terrestrial solutes. Spatial patterns showed elevated dissolved organic carbon (DOC) and trace metal concentrations at agricultural–treed (Ag-Tr) sites, reflecting strong terrestrial organic matter inputs, while Ni concentrations were higher and more variable at downstream and outlet locations. Multivariate analyses demonstrated strong co-variation between DOC and several trace metals, supporting DOM-mediated transport. FT-ICR-MS revealed that DOM was dominated by oxygen rich aromatic compounds, with Ni-associated molecular formulas enriched in heteroatom containing species (e.g., N- and S-bearing compounds) near the outlet, suggesting distinct complexation environments compared to other metals (e.g., Fe, Al) that preferentially associate with oxygen-rich ligands. These findings indicate that hydrologically driven export of terrestrial DOM governs trace metal mobility, while shifts in DOM composition and heteroatom content influence metal-specific transport pathways, particularly for Ni in downstream environments.

T740416

THESE CANS ARE FULL OF CARP! ACCELERATED AGING AND METAL MIGRATION IN CANNED SEAFOOD. **Elaine Lamoureux***[1]; Rachida Chekri [2]; Nathalie Marchond [2]; Clément Mazurais [2]; Petru Jitaru [2]; and Nausheen Sadiq [1]. [1] Mount Royal University, Department of Chemistry, 4825 Mount Royal Gate SW, Calgary, AB T3E 6K6, Canada; [2] ANSES, Laboratory for Food Safety, Trace elements and nanomaterials unit, 14 rue Pierre et Marie Curie, 94700 Maisons-Alfort, France. (elamo968@mtroyal.ca).

Canned seafood is widely consumed due to its affordability and nutritional value [1–3]. However, due to the intrinsic presence of metals in fish, it is important to discern contributions of toxic and persistent elements such as As, Cd, Hg, and Pb from cans [2]. This study examined the effects of

storage time and matrix composition on metal leaching in canned seafood using accelerated aging and ICP-MS. Samples (in original, closed cans) were heated at 65 °C for up to 20 days (simulating ~2 years of storage), and 16 elements were quantified. Results showed increases of 25–50% for most elements, with Co, Cd, and Ba exceeding 100%, however Fe and Sn decreased slightly. Matrix effects were observed, with Pb favoring oil and Cd favoring aqueous media. After 20 days, Hg in several samples and total As in sardines and shrimp exceeded Canadian regulatory limits. These results demonstrate that storage conditions and packing medium significantly influence metal migration, raising concerns about long-term exposure from canned seafood.

T930111

A NOVEL SUPERVISED LEARNING APPROACH FOR THE REAL-TIME OPTIMIZATION OF MASS SPECTROMETRY DATA ACQUISITION INCREASES PROTEOME COVERAGE. **Mathieu Lavallée-Adam***[1]; Iryna Abramchuk; Yun-En Chung [2]; Alona Petrova [3]; Jonathan St-Germain [4]; Jens Decker [5]; Brian Raught [6]; Jonathan Krieger [7]; Tharan Srikumar [8]. [1] University of Ottawa, Department of Biochemistry, Microbiology and Immunology, 451 Smyth Road, Ottawa, ON, K1H 8M5, Canada; [2] University of Ottawa, Department of Biochemistry, Microbiology and Immunology, 451 Smyth Road, Ottawa, ON, K1H 8M5, Canada; [3] University of Ottawa, Department of Biochemistry, Microbiology and Immunology, 451 Smyth Road, Ottawa, ON, K1H 8M5, Canada; [4] University of Ottawa, Department of Biochemistry, Microbiology and Immunology, 451 Smyth Road, Ottawa, ON, K1H 8M5, Canada; [5] Princess Margaret Cancer Centre, 101 College Street, Toronto, ON, M5G 1L8, Canada; [6] Bruker Daltonics GmbH & Co. KG, Fahrenheitstraße 4, Bremen, 28359, Germany; [7] Princess Margaret Cancer Centre, 101 College Street, Toronto, ON, M5G 1L8, Canada; [8] Bruker Ltd, 2800 High Point Dr., Milton, ON, L9T 5V7, Canada. (mathieu.lavallee@uottawa.ca).

While mass spectrometry data-independent acquisition has improved protein identification, data-dependent acquisition (DDA) remains valuable for proteomics applications such as multiplexed samples and crosslinked peptide analyses. However, DDA collects redundant mass spectra from abundant proteins, leaving many low-abundance proteins uncharacterized. We previously presented a software tool (MealTime-MS) that prevents, in real-time, redundant data acquisition from proteins confidently identified during an experiment. Nevertheless, MealTime-MS was only evaluated in simulations. Herein, we present MealTime-MS-2.0, which controls data acquisition on Bruker timsTOF mass spectrometers. The tool uses machine learning to assess, on-the-fly, the confidence of a protein identification based on mass spectra collected for it. Peptides from confidently identified proteins are then excluded from further data collection, allowing the instrument to acquire data from less abundant proteins. MealTime-MS-2.0 data acquisition was compared with a state-of-the-art DDA-PASEF workflow using a K562 whole-cell digest. Experiments guided by MealTime-MS-2.0 identified up to 17.5% more proteins than DDA experiments and 601 proteins not observed with DDA. Proteins identified with MealTime-MS-2.0 exhibit lower abundance than those detected with DDA, suggesting that MealTime-MS-2.0 improves the identification of low-abundance proteins. Overall, MealTime-MS-2.0 allocates mass spectrometry resources more efficiently and detects more low-

abundance proteins than state-of-the-art approaches, improving sample biological characterization.

T92085

SPECIATION OF ARSENIC AND SELENIUM IN FRESHWATER FISH. **Chester Lau***; Hailey Yu; Xiufen Lu; Karen S. Hoy, Wei Chi; Tetiana Davydiuk; Mason D'Souza; Juanjuan Fu; Kade Shepherd; 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, Canada, T6G 2G3 (xcle@ualberta.ca).

Fish provides necessary nutrients in many regions around the world. Marine organisms are known to contain relatively high concentrations of arsenic, mostly in the form of arsenobetaine (AsB). But there have been limited studies on arsenic and selenium species in freshwater fish. Quantification of arsenic and selenium species in freshwater fish requires highly sensitive analytical techniques because of the relatively lower concentrations of arsenic and selenium species in freshwater fish. We report on methods for arsenic and selenium speciation analysis, involving extraction of arsenic and selenium from fish tissues, followed by chromatographic separation and mass spectrometry detection of arsenic and selenium species. We show an application of an arsenic speciation method to the determination of arsenic species in 1643 fish samples, representing 14 common fish species from 53 waterbodies in Alberta, Canada. The total arsenic concentrations in fish ranged from 2.8 to 1200 µg/kg (in wet weight of sample) (mean 71 ± 101 µg/kg), which are all below the 2000 µg/kg (wet weight) maximum allowable total arsenic in fish, recommended by the Ontario Ministry of the Environment. The concentrations of arsenic species in the 1643 fish samples ranged from below the method detection limit of 0.25 µg/kg to the maximum concentrations of 380 µg/kg for AsB, 150 µg/kg for dimethylarsinic acid (DMA), 70 µg/kg for inorganic arsenate (iAsV), and 51 µg/kg for monomethylarsonic acid (MMA). AsB made up 46.1% ± 26.2% of total arsenic species. We also show the determination of selenite [Se(IV)], selenate [Se(VI)], selenocystine (SeCys2), methylselenocysteine (MetSeCys), and selenomethionine (SeMet) in brown trout, lake trout, and mountain whitefish. SeMet was the main selenium species, with concentrations ranging from 1120 µg/kg to 3771 µg/kg (mean 2745 ± 861 µg/kg), accounting for (93.2 ± 1.4)% of total selenium. Inorganic selenium Se(IV) and Se(VI) were at trace concentrations, ranging from below detection limit to 32.5 µg/kg (mean 21.5 ± 10.9 µg/kg). The concentration and speciation information obtained from this research is critical for assessing environmental impact and biotransformation of arsenic and selenium species in aquatic ecosystems.

T81042

CADMIUM AND LEAD IN CACAO POWDER: AN INTERNATIONAL INTER-COMPARISON EXERCISE AND DEVELOPMENT OF A CERTIFIED REFERENCE MATERIAL. **Kelly LeBlanc***; Kenny Nadeau; Calvin

Palmer; Enea Pagliano; Lu Yang; long Grinberg. Metrology Research Centre, National Research Council Canada. (kelly.leblanc@nrc-cnrc.gc.ca).

Concerning levels of toxic metals found in chocolate have prompted some recent changes to the maximum allowable content in commercial goods worldwide. Cadmium and lead are the elements of greatest interest in cacao products and have the potential to be detrimental to health even when consumed in trace amounts. Among the tools required for regulatory compliance are analytical methods capable of accurate, precise, and SI-traceable measurements of cadmium and lead in cacao-based matrices, and Certified Reference Materials that aid in validating these methods. In support of this endeavour, we recently organized an international intercomparison exercise within the Inter-American Metrology System (or SIM, Sistema Interamericano de Metrología), examining the cadmium and lead content in a sample of cacao powder. Nineteen institutes from within SIM as well as the broader metrology community participated in the comparison. This talk will discuss the challenges faced during sample analysis and in arriving at consensus values for cadmium and lead content in this unique matrix, and will outline the importance of such intercomparisons to the metrology community.

T82056

INVESTIGATING ELECTROCHEMILUMINESCENCE OF GOLD NANOCLUSTERS THROUGH ADVANCED SPECTROELECTROCHEMISTRY. **Ian Lee***; Ruizhong Zhang; Zhifeng Ding. Western University, Department of Chemistry, 1151 Richmond St, London, ON N6A 3K7, Canada. (ilee87@uwo.ca).

Gold NCs have become prominent as versatile emitters for electrochemiluminescence (ECL), due to their rich valence states, atomically precise structures, and tunable electronic properties. As an analytical method, ECL has attracted much attention for its applications in optical imaging and immunoassays, due to unique features like wide dynamic detection range, low background signals and no need for external light source [1]. Preliminary results of electrochemistry and ECL experiments revealed Au3 and Au19Cu3 NCs' promising emissive properties in this research, showcased by the absolute quantum efficiencies measured through novel method previously reported by our group [2]. Furthermore, the emission behaviors of the nanoclusters were examined through applications of laser-induced photoluminescence and advanced ECL spectroscopy techniques . Through spectroelectrochemical methods, emission changes can be monitored, enabling simultaneous studies of the redox and excited state species in real time. The resulting spectra demonstrated shifting emission wavelengths, indicating formation of different excited species and providing insight into the mechanisms of the ECL reactions.

T72007

(2026 BURGENER RESEARCH GRADUATE STUDENT TRAVEL AWARD LECTURE) ELECTROCHEMICAL CONVERSION OF SUBSTITUTED PHENOLS. **Tyra Lewis***[1]; Dr. Sanela Martic [2,3]. [1] Materials Science; [2] Environmental and Life Sciences; [3] Department of Forensic Science, Trent University, Peterborough, ON Canada. (tyralewis@trentu.ca).

Phenolic compounds have application in biotechnology and agriculture industries and may be reintroduced into the environment as waste. The conversion of phenolic pollutants is traditionally achievable using harsh chemical treatments. However, the selective conversion of phenolics into new functional molecules can also be achieved using milder, greener and more sustainable avenues such as electrosynthesis [1]. The electrochemical oxidation of phenolic compounds generates a variety of products, including quinones, polymers and new carbon carbon bonds, further resulting in the synthesis of new value-added chemicals of industrial interest. Herein, the electrochemical conversion of 2,6-di-tert-butylphenol (DTBP), 2,6- diphenylphenol (DPP), and 5-chloro-2-(2,4-dichlorophenoxy)phenol (triclosan) were compared to a traditional chemical oxidation process [2,3]. All compounds underwent conversion during cyclic voltammetry (CV) or after addition of an oxidizing agent and resulted in significant colour changes. The product formation was monitored by UV-Vis spectroscopy and further characterized by single crystal X-ray diffraction (SC-XRD) and gas chromatography-mass spectrometry (GC-MS). Carbon-carbon bond dimerization was uniquely observed when dimer was formed. Overall, the data suggested that the product yield and the selectivity of electrosynthesis were dependent on the parameters and substrate used, and that electrosynthesis may allow for reaction selectivity and yield, which is not conventionally achievable by chemical means.

T81051

DISTINCT ELECTROCHEMICAL AND CATALYTIC PROPERTIES OF ELECTRODEPOSITED AND DROP-CASTED GOLD NANOPARTICLES. **Tyra Lewis***[1]; Sanela Martic [2,3]. [1] Materials Science; [2] Environmental and Life Sciences; [3]Department of Forensic Science, Trent University, Peterborough, ON Canada. (tyralewis@trentu.ca).

Phenolic compounds have application in biotechnology and agriculture industries and may be reintroduced into the environment as waste. The conversion of phenolic pollutants is traditionally achievable using harsh chemical treatments. However, the selective conversion of phenolics into new functional molecules can also be achieved using milder, greener and more sustainable avenues such as electrosynthesis [1]. The electrochemical oxidation of phenolic compounds generates a variety of products, including quinones, polymers and new carbon carbon bonds, further resulting in the synthesis of new value-added chemicals of industrial interest. Herein, the electrochemical conversion of 2,6-di-tert-butylphenol (DTBP), 2,6- diphenylphenol (DPP), and 5-chloro-2-(2,4-dichlorophenoxy)phenol (triclosan) were compared to a traditional chemical oxidation process [2,3]. All compounds underwent conversion during cyclic voltammetry (CV) or after addition of an oxidizing

agent and resulted in significant colour changes. The product formation was monitored by UV-Vis spectroscopy and further characterized by single crystal X-ray diffraction (SC-XRD) and gas chromatography-mass spectrometry (GC-MS). Carbon-carbon bond dimerization was uniquely observed when dimer was formed. Overall, the data suggested that the product yield and the selectivity of electrosynthesis were dependent on the parameters and substrate used, and that electrosynthesis may allow for reaction selectivity and yield, which is not conventionally achievable by chemical means.

T730114

MICRO-TECHNOLOGIES FOR EXTRACELLULAR VESICLE ISOLATION AND ANALYSIS. Roshan Tosh Aggarwal; Lian Miller; Isabella Walker; **Huiyan Li***. College of Engineering, University of Guelph, 50 Stone Rd E, Guelph, ON N1G 2W1, Canada. (huiyanli@uoguelph.ca).

Extracellular vesicles (EVs) are important mediators of intercellular communication and hold significant promise as biomarkers for disease diagnosis and monitoring. However, efficient isolation and sensitive analysis of EVs remain major challenges due to their small size, heterogeneity, and low abundance in biological samples. This talk will introduce two complementary micro-technologies developed in our laboratory to improve the specificity, sensitivity, and throughput of EV analysis. First, micro-bead–based platforms will be presented for highly specific EV isolation and highly sensitive EV quantification. Second, a microarray-based technology will be discussed for convenient and multiplexed quantification of EV proteins. By establishing a new microarray format, this platform enables simultaneous measurement of multiple EV protein markers, facilitating low-cost high-throughput EV profiling. Together, these micro-technologies provide versatile approaches for EV isolation and analysis with improved sensitivity, specificity, and multiplexing capability, offering promising tools for EV-based biomarker discovery.

T730115

DISCOVERY OF HIDDEN N-DIMETHYLAMINE PRECURSORS. Tingting Zhao [1]; Menglan Gao [1,2]; Xiaobin Liao [2]; **Xing-Fang Li***[1]. [1] Division of Analytical and Environmental Toxicology, University of Alberta; [2] Huaqiao University, Xiaomen, China (xingfang.li@ualberta.ca).

Water disinfection ensures drinking water safety by inactivating pathogens but can also produce toxic byproducts like nitrosamines from reactions with organic matter. Among ~700 identified DBPs, NDMA is a carcinogenic compound formed from nitrogen-containing organics. Identifying its precursors is key to controlling its formation. While past research has focused on dimethylamine (DMA)-containing compounds, we hypothesize that NDMA can also form from nitrogen compounds without DMA. To confirm this, we started our investigation by analyzing experimental MS/MS spectra of 39 known NDMA precursors. Using the observed fragmentation patterns of these known

precursors, we queried the NIST 23 MS/MS library, which contains high-resolution mass spectra for a wide range of compounds, to identify potential NDMA precursors. To facilitate large-scale screening, we integrated these rules into a bioinformatic tool, NitrosAmine Precursor eXplorer (NitraPreX) to identify potential NDMA precursors in nontargeted LC-HRMS analysis. The performance of NitraPreX was evaluated by conducting chloramination on the discovered new NDMA precursors and confirming their NDMA formation potential.We identified and applied three diagnostic fragment ions [C2H6N]+, [C2H7N]·+, and [C2H8N]+to search the NIST23 MS/MS library, and discovered new NDMA candidates. Seven commercially available compounds were experimentally confirmed as NDMA precursors (four with DMA moieties and three without), along with five additional non-DMA-containing drugs. Notably, hydroxychloroquine and chloroquine, despite lacking DMA, showed higher NDMA yields than the DMA-containing precursors. This approach complements traditional DMA based methods and enables discovery of previously overlooked precursors, including those without DMA or with unknown structures. Using NitraPreX to analyze standard reference materials and real water samples, we identified over 200 potential NDMA precursors, demonstrating a new tool for nitrosamine research.

T741016

APPLICATION OF METAL NANOPARTICLES FOR HIGHLY SENSITIVE AND CONVENIENT ANALYSIS OF CELLS AND EXTRACELLULAR VESICLES. **Huiyan Li***; Rebecca Goodrum; Kara Cook. College of Engineering, University of Guelph, 50 Stone Rd E, Guelph, ON N1G 2W1, Canada (huiyanli@uoguelph.ca).

Protein quantification in cells and extracellular vesicles (EVs) provides important insights into health and disease. While immunoassays are widely used for protein detection, conventional assays often lack the sensitivity required to detect low-abundance biomarkers for early diagnosis. In addition, EV particle quantification can reflect disease status, but existing methods typically rely on complex and costly instrumentation, creating a major bottleneck in EV analysis. To address these challenges, our laboratory has developed sensitive and easy-to-implement platforms for protein and EV quantification using metal nanoparticles. These nanoparticles enable both fluorescence signal amplification and colorimetric detection. For protein quantification in cells and EVs, the fluorescence-based platform achieves limits of detection that are 3–4 orders of magnitude lower than those of conventional immunoassays. For EV quantification, we developed a simple colorimetric assay that can be read using a standard 96-well plate reader. These platforms provide accessible and highly sensitive analytical tools for biomarker discovery and validation in disease diagnostics.

T930114

A VISUALIZATION AND FLUORIMETRIC DETECTION FOR SULFISOXAZOLE BASED ON SELECTIVELY WEAKENED PEROXIDASE ACTIVITY OF GOLD NANOCLUSTERS. **Meiling Li [1,2,3]; Huaidong Peng [4]; Yanlan Liang; Jiang Meng [1]; Hongliang Huang; Paul C.H. Li***[5]; Yue Sun [1,2,3]. [1] School of Traditional Chinese Medicine, Guangdong Pharmaceutical University, Guangzhou 510006, China; [2] Key Laboratory of State Administration of TCM for Digital Quality Evaluation of Chinese Materia Medica, Guangzhou 510006, China; [3] Engineering & Technology Research Center for Chinese Materia Medica Quality of Guangdong Province, Guangzhou 510006, China; [4] Department of Pharmacy, The Second Affiliated Hospital of Guangzhou Medical University, Guangzhou 510260, China; [5] Department of Chemistry, Simon Fraser University, Burnaby, BC V5A 1S6, Canada (paulli@sfu.ca).

In this study, a facile method to detect sulfisoxazole (SFX) sensitively and selectively was developed by use of BSA-stabilized Au nanoclusters (BSA-AuNCs). These nanoclusters, which possess high intrinsic peroxidase-like activity, can catalyze hydrogen peroxide (H2O2)-based oxidation of o-phenylenediamine (OPD) and to rapidly generate bright yellow 2,3-diaminophenazine. We have found that the antibiotics SFX can strongly inhibit the catalytic activity of BSA-AuNCs, while other common sulfonamide compounds do not interfere. As the concentration of SFX increases, the system yellow color produced can be weakened, and this becomes lightened to colorless to achieve a visual detection of the presence of SFX colorimetrically. The detection limit of this method is as low as 20 nM with the help of UV-vis spectroscopy and 50 nM by naked-eye observation. In addition, the decrease in intensity due to SFX also works in fluorimetry and the detection limit of SFX can be as low as 5 nM. The proposed method is successfully applied for the detection of SFX in meat and mice blood samples after the animals (i.e. chicken, pig) have taken medicated foods. In this study, a facile method for the sensitive and selective detection of sulfisoxazole (SFX) was developed using BSA-stabilized Au nanoclusters (BSA-AuNCs). These nanoclusters, which possess high intrinsic peroxidase-like activity, can catalyze the hydrogen peroxide (H2O2)-based oxidation of o-phenylenediamine (OPD) and rapidly generate bright yellow 2,3-diaminophenazine. We found that the antibiotic SFX strongly inhibits the catalytic activity of BSA-AuNCs, while other common sulfonamide compounds do not interfere. As the concentration of SFX increases, the yellow color produced by the system weakens, eventually fading to colorless, enabling visual detection of SFX colorimetrically. The detection limit of this method is as low as 20 nM using UV-vis spectroscopy and 50 nM by naked-eye observation. In addition, the decrease in intensity due to SFX is also detectable by fluorimetry, with a detection limit as low as 5 nM. The proposed method has been successfully applied for the detection of SFX in meat and blood samples from animals (i.e., chicken, pig) that have consumed medicated food.

T92058

CONTRASTING EFFECTS OF HEMIN AND GO-MPC MODIFIERS ON THE ELECTROCHEMICAL RESPONSE OF Δ9-TETRAHYDROCANNIBINOL. **Dhésmon Lima***; Kaique A. Mendes; Kyle Mosher;

Paige Thornton; Marianna Kovtun; Sarah Mulla. Department of Chemistry and Physics, Mount Saint Vincent University, 166 Bedford Highway, Halifax, NS B3M 2J6, Canada. (dhesmon.lima1@msvu.ca).

Detecting psychoactive drugs in environmental and consumer-relevant samples has become important due to their widespread use and persistence. Electrochemical detection offers low cost, rapid analysis, and high sensitivity; however, responses are governed by electrode surface chemistry and interfacial processes. Two complementary strategies were investigated using Δ9-tetrahydrocannabinol (THC) as a model analyte. First, graphite paste electrodes modified with hemin were studied through optimization of graphite:hemin ratio, solution pH, and voltammetric parameters, with cyclic voltammetry and electrochemical impedance spectroscopy used to probe electron-transfer behaviour. Hemin modification enhanced responses toward both ferricyanide and THC, increasing current and improving signal definition, suggesting redox-mediated interfacial contributions. Second, graphene oxide–metal phthalocyanine (GO–MPc, M=Fe, Co, Ni) conjugates were incorporated into graphite paste electrodes to examine nanostructured interfacial effects arising from GO–MPc integration. Ferricyanide showed enhanced currents and reversibility at modified electrodes, dominated by graphene oxide–induced surface area and charge transport improvements. In contrast, THC oxidation was irreversible and adsorption-controlled, with GO–MPc nanoconjugates providing limited improvement despite increased current, accompanied by peak broadening and anodic shifts. These results demonstrate that enhanced electron-transfer kinetics do not directly translate to improved detection of hydrophobic analytes, emphasizing the need for analyte-specific electrode design.

T72005

(2026 PERKINELMER ANALYTICAL SCIENCES AND SPECTROSCOPY AWARD LECTURE). **Chang Liu***. SCIEX, 71 Four Valley Drive, Concord, ON, Canada L4K 4V8 (chang.liu@sciex.com).

We describe an Acoustic Ejection Mass Spectrometry (AEMS) platform resulting from the integration of acoustic droplet ejection (ADE) technology, an open-port interface (OPI), and electrospray ionization (ESI) MS that creates a novel system enabling high-speed sampling and label-free analysis. The ADE technology delivers nanoliter droplets in a touchless manner with high speed, precision, and accuracy; subsequent sample dilution within the OPI, in concert with the capabilities of modern ESI-MS, minimizes the laborious sample preparation and method development required in current approaches. This AEMS platform has been applied to a variety of drug discovery workflows, including high-throughput (HT) biochemical screening, cell-based screening, covalent binders screening, HT native MS, label-free in situ enzyme kinetics, in vitro and in vivo adsorption, distribution, metabolism, elimination, pharmacokinetic (PK) and biomarker analysis, compound QC, HT parallel medicinal chemistry, and biocatalysis. The system principles and representative applications of the AEMS technology will be discussed in this presentation.

T730411

CHALLENGES AND SOLUTIONS FOR TRACE ELEMENT DETERMINATION IN HIGH-FAT FOOD MATRICES. **Bob Lockerman***; Jessica Giles; Alicia Stell; Layla Abu-Al-Halaweh; Lanie Griffin Hough. CEM Corporation, 3100 Smith Farm Road, Matthews, NC 28104, USA. (bob.lockerman@cem.com).

The varied nature of food matrices presents significant analytical challenges, particularly when detecting environmental contaminants such as trace elements. Among the most concerning are the “big four” toxic heavy metals—arsenic, cadmium, lead, and mercury—which are well documented for their harmful effects on human health. Beyond these heavy metals, there are other elements of importance to human health. As a result, monitoring a variety of elements in food products remains essential for meeting regulatory and safety guidelines. The complexity of some food matrices, such as high-fat foods, makes breaking down the matrix to achieve regulatory levels very challenging. Effective trace element analysis requires a sample preparation method that is reliable, reproducible, and robust, while also being adaptable to a wide variety of food types. In this study, trace element concentrations are measured across a range of high-fat food matrices, including standard reference materials, achieving good recovery and reproducibility. The adaptability of this method is further explored by evaluating a larger sample size and a higher temperature than traditionally used for these high-fat foods. The analysis is performed using ICP-MS following microwave digestion, which offers a fast, efficient, and straightforward approach for detecting trace elements in challenging food samples.

P750125

TIME-RESOLVED ANALYSIS OF TRYPSIN DIGESTION KINETICS USING LC-UV. **Kassandra Lok***; Adam Lynch; Alan Doucette. Department of Chemistry, Dalhousie University, Halifax, NS, B3H 4R2 (ks297360@dal.ca).

Trypsin, a proteolytic enzyme, is widely used for protein digestion in bioanalytical laboratories. While trypsin digestion of complex proteins is extensively studied in the field of mass spectrometry-based proteomics, very few studies have been completed on the optimization of the digestion procedure alone. The efficiency and reproducibility of trypsin digestion depend on several factors, including enzyme-to-substrate ratio, digestion time, and final pH. This study focuses on the time-dependent kinetics of protein digestion by trypsin, performed under controlled conditions, with careful monitoring of the digestion progress by using a time-resolved sampling approach. Aliquots are collected over time ranging from seconds to minutes to hours. Samples are analyzed via liquid chromatography with UV detection, tracking progression through changes in chromatographic peak areas corresponding to the intact protein and its fragmented peptides. This approach enables quantitative evaluation of protein degradation and peptide formation as a function of time, allowing for the identification of the time required to reach digestion completion. In addition, the influence of enzyme-to-substrate ratio and stopping agent pH on digestion efficiency is assessed. The results of this study provide insight into the kinetics of trypsin-mediated digestion and contribute to the

optimization of digestion protocols for simple proteins. Improved control over digestion conditions can enhance reproducibility and reduce waste in analytical laboratories.

T71004

(2026 UNDERGRADUATE STUDENT TRAVEL AWARD LECTURE) INVESTIGATING CANCER THROUGH THE LENS OF TRYPTOPHAN METABOLISM. **Kara Loudon***; Maria Penagos Gonzalez; Michael Saley; Sabine Kuss. Laboratory for Bioanalytics and Electrochemical Sensing, University of Manitoba, Department of Chemistry, 144 Dysart Road, Winnipeg, MB R3T 2N2, Canada. (loudonk@myumanitoba.ca).

Shedding new light on cancer metabolism, we applied electrochemistry to understand the relationship between the tryptophan - kynurenine (trp – kyn) metabolic pathway and cancer treatment. Glioblastoma is an aggressive brain cancer that impacts Canadians, placing significant strain on our healthcare systems. Treatment of this cancer is complicated by mechanisms through which it can evade detection, including an upregulation of trp catabolism through the kyn pathway. Previous research has focused on inhibition of the enzymes that catalyze this pathway, however it was observed that select inhibition of one enzyme can cause compensatory upregulation of another. This suggested that dual inhibition was necessary, and clinical trials are underway using such inhibitors. In this work, we employed the powerful electroanalytical techniques Voltammetry and Scanning Electrochemical Microscopy to define the electrochemical fingerprint of trp, elucidate optimal experimental conditions and probe the conversion of trp to kyn in cancer cells. Future work aims to treat this cell line with dual inhibitors and determine the corresponding changes in trp metabolism. Our results therefore highlight the potential of electrochemical approaches to assess the efficacy of dual inhibitors of the trp – kyn pathway.

P750947

EVALUATION OF EXTRACTION TECHNIQUES FOR ARSENIC SPECIATION IN FISH. **Xiufen Lu***; Quinn Goldberg; X. Chris Le. Division of Analytical and Environmental Toxicology, Department of Laboratory Medicine and Pathology, Faculty of Medicine and Dentistry, University of Alberta, Alberta T6G 2G3, Canada (xlu@ualberta.ca).

Arsenic is a naturally occurring element found in the earth's crust and can enter groundwater systems through both natural processes and human activities. A variety of arsenic species may be present in fish. The objective of this research is to evaluate different extraction methods for the determination of arsenic species in fish. Brown trout, Lake trout, and Mountain whitefish were collected from Crowsnest Lake in Alberta, and arsenic species were extracted from their muscle tissue using either a 50/50 methanol–water solution or an enzyme-assisted extraction with sonication. Overall, the enzyme-assisted extraction yielded higher concentrations of extracted

arsenic species. The arsenic species in the extracts were separated using anion-exchange high-performance liquid chromatography (HPLC) and detected using inductively coupled plasma mass spectrometry (ICP-MS). Arsenobetaine (AsB) constituted the majority of the arsenic species in lake trout and brown trout, while inorganic arsenic (iAsV) was the predominant species in mountain whitefish. Dimethylarsinic acid (DMA) and monomethylarsonic acid (MMA) were detected in most of the fish species at low concentrations. Inorganic arsenic (iAsIII) was not detectable in any samples using the methanol–water method, but low concentrations were detected using the enzymatic method. Three unknown arsenic species were also observed. Both enzyme-assisted extraction and the method of methanol-water extraction are useful for arsenic speciation analysis.

P750121

INVESTIGATING AMINO ACID CONTRIBUTIONS TO IN-SOURCE FRAGMENTATION IN ELECTROSPRAY IONIZATION MASS SPECTROMETRY. **Adam Lynch***; Alan Doucette; Carlie Charron. Department of Chemistry, Dalhousie University, Halifax, NS, B3H 4R2 (ad647601@dal.ca).

Mass spectrometry is widely regarded as the gold standard for analytical measurements; however, it is not without limitations. Although electrospray ionization (ESI) is considered a soft ionization technique, certain operating conditions can introduce complications, including in-source fragmentation (ISF). ISF occurs when ions fragment within the ion source prior to entering the mass analyzer and undergoing MS/MS fragmentation. This phenomenon can arise under a variety of ESI conditions, such as elevated spray voltages, aggressive gas flows, and excessively high source temperatures.In extreme cases, ISF has been reported to account for up to nearly 60% of identified peptides in standard mixtures. [1] Despite the diversity of sequences observed in tryptic peptides, there remains a limited understanding of how specific amino acid bonds respond to these ionization conditions. We propose that a deeper understanding of amino acid–dependent fragmentation behavior in the ion source will improve peptide identification workflows, enabling more accurate database searching and reducing false-positive identifications.

T730514

TRACKING CARBOPLATIN CHEMORESISTANCE IN OVARIAN CANCER BY SCANNING ELECTROCHEMICAL MICROSCOPY. **Mengzhen Lyu***[1]; Roy Daou [1]; Katherine Bazin [1]; Dao Trinh [2]; Michael A. Saley [1]; Dhésmon Lima [1,3]; Mark W. Nachtigal [4]; Sabine Kuss [1]. [1] Laboratory for Bioanalytics and Electrochemical Sensing, Department of Chemistry, Faculty of Science, University of Manitoba, 144 Dysart Road, Winnipeg, Manitoba, Canada, [2] Laboratoire des Sciences, de l'Ingénieur pour l'Environnement (LaSIE) UMR CNRS 7356, Université de La Rochelle, Pôle Sciences et Technologie, Avenue Michel Crépeau, Cedex 1, La Rochelle, France, [3] Department of Chemistry and Physics, Mount Saint Vincent University, 166 Bedford Highway, Halifax, NS, Canada,

[4] Department of Biochemistry and Medical Genetics, Rady Faculty of Health Sciences, University of Manitoba, 745 Bannatyne Avenue, Winnipeg, Manitoba, Canada (lyum@myumanitoba.ca).

Cancer drug resistance remains a major challenge in oncology and contributes to many chemotherapy failure[1]. Ovarian cancer is commonly treated with platinum-based agents such as carboplatin (CBDCA); however, chemoresistance rates are increasing annually. The exact underlying platinum resistance mechanisms are not fully understood, and there is a need for analytical methods to identify resistant mechanisms. Here, we develop a scanning electrochemical microscopy (SECM)-based approach for chemoresistance detection through quantifying glutathione (GSH), a major cell metabolite associated with drug resistance[2]. This presentation reports studies on carboplatin-sensitive and -resistant A2780 model cell lines of ovarian cancer, as well as patient-derived ovarian cancer cell lines PEO1, PEO4, and PEO6. SECM reveals distinct metabolic responses across cell lines upon carboplatin exposure. Overall, this study highlights the potential of electrochemistry to detect chemotherapy-resistant phenotypes in cell samples and the investigation of resistance mechanisms in living cells by electrochemistry.

T830315

ACCURATE SEX DETERMINATION THROUGH MULTI-ELEMENTAL ANALYSIS OF FINGERNAILS USING ELECTROTHERMAL VAPORIZATION COUPLED TO INDUCTIVELY COUPLED PLASMA OPTICAL EMISSION SPECTROMETRY. **Margaret MacConnachie***; Andrew Schug; Diane Beauchemin. Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada (mmacconnachie@mtroyal.ca).

Within forensic science, the analysis of trace evidence is vital. Though they can be useful, biological materials such as blood, sweat, and saliva, typically degrade rapidly. Keratin-based tissues, such as hair and nails, offer a substantially more stable alternative. Here, an established method for accurate sex determination in humans via the multi-elemental analysis of head hair[1], in combination with multivariate statistics, was applied for the first time to fingernail samples. Multi-elemental analysis of fingernail samples was performed by solid sampling electrothermal vaporisation (ETV) coupled to inductively coupled plasma optical emission spectrometry (ICPOES). Nail samples were washed in acetone, followed by doubly deionized water, and air dried prior to analysis via ETV-ICPOES; only 2 mg of nail tissue is required for analysis. Point by-point internal standardization was performed to compensate for sample loading effects on the plasma. Peak areas were integrated and mass corrected before statistical analysis. Multivariate analysis was used for sample classification; although principal component analysis provided insufficient separation between the sexes, linear discriminant analysis was highly effective for sex determination. This work paves the way for broader use of multi-elemental sex determination methods within forensic science.

P750642

PHOTOREMEDIATION OF PHARMACEUTICAL WASTE: A LIGHT-ACTIVATED APPROACH TO WATER DECONTAMINATION. **Ella MacPhee***[1]; Sydney Palmer [1]; Marzi Baneshi [2]; Stephanie MacQuarrie [2]; Geniece Hallett-Tapley [1]. [1] St. Francis Xavier University, Department of Chemistry, 5009 Chapel Sq., Antigonish, NS B2G 2W5; [2] Cape Breton University, Department of Chemistry, 1250 Grand Lake Rd., Sydney, NS B1M 1A2 (x2023aph@stfx.ca).

Global water remediation is driven by increasing contamination from industrial effluents and improper pharmaceutical disposal. Traditional routes of pollutant decontamination, such as filtration, chemical/biological treatments, and incineration, are invasive and often fail to achieve full removal. Heterogenous materials have gained attention, with many relying on the semiconductor activity of TiO2 and ZnO to solve these issues. The proposed research will showcase the benefit of gold nanoparticle (AuNP)-modified TiO2 and ZnO/biochar materials (Figure 1) to establish environmentally favourable treatment routes for pharmaceutical waste, with focus on estradiol, common in many hormone treatment therapies, as well as Atenolol, used it the treatment of hypertension and Penicillin G, a common antibiotic. Improper disposal or incomplete metabolism of these pharmaceuticals has been implicated in many current health and environmental issues, such as breast cancer, hormonal imbalances, feminization of aquaculture and antibiotic resistance. Key targets for material optimization include nanoparticle shape and biochar origin. Biochar, used in conjunction with the MacQuarrie Research Group at Cape Breaton University, is a carbon-rich, porous solid generated from the high-temperature treatment of forestry and seafood-processing waste. Its ability to improve the adsorption capacity of the catalyst system by trapping the chosen pollutant will be examined as a key advancement in photocatalytic pollutant remediation strategies

T82025

NANOPLASMONIC MICROFLUIDICS FOR ENHANCED CHARGE-TRANSFER KINETICS IN CLINICAL DIAGNOSTICS. **Sara Mahshid***. Department of Bioengineering, McGill University, Montreal, Quebec, Canada (sara.mahshid@mcgill.ca).

Development of diagnostic devices with clinically relevant sensitivity and rapidity is highly desirable for decreasing the delay between diagnosis and treatment. Diagnostic inefficiency permeates multiple medical fields, including infectious diseases and cancer. In the Mahshid Lab, we develop next-generation diagnostic technologies and health monitoring that integrate smart nanomaterials, pocket-sized microfluidic devices, and machine learning to detect disease hallmarks. From an engineering perspective, the lab seeks to develop novel plasmonic nanomaterials with intrinsic opto-electrical properties for amplifying detection signals across different read-outs, enabling ultra-rapid identification of disease-driving biomolecules in complex biological samples (e.g. in blood, saliva and urine). The miniaturized nano-sensors can be integrated into automated lab-on-a-chip platforms capable of operating with small sample volumes and precise reagent dosing, facilitating the transition to portable diagnostic tools. The proposed hybrid devices could be deployed as portable

tools for in-field testing, remote locations and hospitals. From a health industry perspective, these devices impact multiple medical fields, including infectious diseases, where rapid diagnosis in minutes rather than hours can reduce transmission, and cancer, where therapies often lag behind disease complexity. They can also enable cancer patients to monitor early stages of tumor recurrence. Additionally, the application of such devices addresses the antimicrobial resistance (AMR) crisis, where the rapid emergence of resistance against first-line antibiotics undermines empirical treatment strategies. Our work on 'smart' plasmonic nanopatterns led to the discovery of plasmonic hot-spot catalysis, which accelerates nucleic acid amplification and enables colorimetric quantification for DNA and RNA targets from pathogens. We also developed plasmonic nanocavity platforms for generating unique Raman spectra that capture the biochemical complexity of cancer biomarkers carried by extracellular vesicles (EV's).

T840218

RAPID DIAGNOSTICTECHNOLOGIES FROM CONCEPTUALIZTION TO COMMERCIALIZTION : A JOURNEY FOR QOLOREX. **Sahar Mahshid***. Department of Bioengineering, McGill University, Montreal, Quebec, Canada (sahar.mahhsid@beetabiomed.com).

Rapid identification of infectious pathogens and their antimicrobial resistance (AMR) signatures is essential for guiding timely, targeted treatment and preventing the spread of resistant organisms. Delays in both pathogen detection and AMR profiling contribute to inappropriate antibiotic use, worsening resistance trends, and increased morbidity—particularly in decentralized or resource-limited settings. Current PCR-based diagnostics, while highly accurate, require multi-step workflows, specialized personnel, and complex instrumentation, limiting their ability to deliver rapid, actionable results at the point of care. QolorEX and its PLUS platform overcome these limitations through a fully automated, cartridge-based system that integrates plasmonic nanostructures, microfluidic automation, and AI-enhanced spectral analysis to deliver multiplexed molecular detection and AMR assessment in under 30 minutes. The platform performs direct-from-sample analysis without manual extraction or amplification steps, enabling simultaneous identification of viral, bacterial, and fungal pathogens alongside genotypic and phenotypic AMR markers. This dual-capability approach supports antimicrobial stewardship by enabling clinicians to select the right therapy on the first encounter.Developed through a translational partnership between McGill University’s Mahshid Lab and affiliated hospitals, QolorEX is advancing toward clinical validation and manufacturable deployment through Beeta Biomed. By unifying speed, automation, multiplexing, and AMR testing, QolorEX and its PLUS platform represent a next-generation solution for decentralized diagnostics and real-time resistance surveillance.

P750643

FUNCTIONALIZATION OF TITANIUM DIOXIDE NANOPARTICLES WITH ANTIOXIDANT-CHITOSAN MATERIALS FOR ANTI-AGING APPLICATIONS. **Makayla Bugden***;Sasha MacDonald; Geniece Hallett-Tapley. St. Francis Xavier University, Department of Chemistry, 5009 Chapel Square, Antigonish, NS B2G 2W5, Canada. (x2023dfh@stfx.ca).

Age-related tissue degradation is closely correlated with prolonged exposure to environmental stressors, including ultraviolet (UV) radiation, which can induce oxidative stress at the cellular level. Aging is characterized by a gradual decline in cellular structure and function, driven in part by the accumulation of reactive oxygen species (ROS). Oxidative stress arises from an imbalance between ROS generation and antioxidant defense mechanisms, leading to damage of critical biomolecules such as lipids, proteins, and nucleic acids. Titanium dioxide (TiO_2) is widely used in sunscreen and biomedical applications due to its chemical stability, low cost, and strong photocatalytic activity; however, UV-activated TiO_2 can generate ROS, potentially exacerbating oxidative damage to surrounding tissues. Incorporating antioxidant interlayers within TiO_2 represents a promising strategy for mitigating ROS formation while preserving material performance. Additionally, surface functionalization with chitosan—a biocompatible, biodegradable polysaccharide—can reduce direct exposure to reactive surfaces while imparting antibacterial functionality. This presentation will discuss initial results from the functionalization of TiO_2 nanoparticles with commercially available antioxidants and evaluate their ability to subdue UV-induced ROS generation. Subsequent chitosan derivatization is expected to enhance biocompatibility and antibacterial performance, advancing hybrid nanomaterials for next-generation sun-protection and anti-aging cosmetic applications.

T840716

STRUCTURAL BASIS OF RECEPTOR RECOGNITION AND IMMUNITY IN THE GARVICIN Q BACTERIOCIN SYSTEM. **T. Mallett***; T. Lamer; J.C. Vederas. Department of Chemistry, University of Alberta, Edmonton, AB, Canada (mallett1@ualberta.ca).

Antimicrobial resistance (AMR) poses a growing global health threat, driving the need for new antimicrobial strategies. (1) Bacteriocins, ribosomally synthesized antimicrobial peptides, are promising alternatives due to their potency, selectivity, and potential for rational engineering. (2) Garvicin Q (GarQ), produced by Lactococcus garvieae, is a bacteriocin that acts on the mannose phosphotransferase system (man-PTS) and is notable for inhibiting priority pathogens, including Listeria monocytogenes and Enterococcus spp. (3,4) To prevent self-toxicity, the GarQ immunity protein GarI acts intracellularly by displacing GarQ from the man-PTS. (5) However, the molecular basis of GarQ-GarI immunity and the determinants of GarQ's unusually broad activity have only recently been investigated. Solution NMR studies from our group revealed that GarQ adopts a distinctive dual-α-helical fold in solution, and that GarI is a structurally dynamic protein featuring an α-helical bundle. (6) In contrast, recent cryo-EM structures of GarQ bound to the man-PTS reveal a markedly different receptor-bound architecture, highlighting key receptor mediated interactions. (7)

Together, these findings provide insight into GarQ conformational remodelling, receptor recognition, and immunity, informing its development as a therapeutically relevant antimicrobial scaffold.

T82098

THE ROLE OF ALGAE BLOOMS AND INORGANIC CONTAMINANT CYCLING ALONG LAKE ERIE SHORELINES. **Vaughn Managl***. Brock University; Chemistry Department, 500 Glenridge Avenue, St. Catharines, Ontario L2S 3A1, Canada (vmangal@brocku.ca).

In southern Ontario, high nutrient runoff from agricultural activities, coupled with warm summer waters, has led to recurring algal blooms in the Great Lakes, especially Lake Erie. Recent findings have begun to explore the interconnected relationship between algae and how the surrounding redox environment, rich in organic matter and low in oxygen, facilitates the biotic methylation of inorganic mercury to the neurotoxin methylmercury. Despite these recent advances, these patterns and variability across algae blooms in Lake Erie have not been explored. In this study, mercury and methylmercury concentrations during Cladophora blooms in Lake Erie were assessed, along with changes in water quality, high-resolution mass spectrometry of organic matter, and proteomics to examine how methylmercury is cycled at three beaches during the summer months of 2024-2025. Filtered mercury concentrations peaked in July at 0.3 ng/L, whereas unfiltered mercury concentrations peaked in August at 1.6 ng/L. High-resolution mass spectrometry revealed a pulse of small amino acids, simple lipids, and phosphorus during a summer storm event, which coincided with increased algae biomass and reduced dissolved oxygen. To further reinforce the role of microorganisms in the methylation process, genetic analyses are in progress, using primers targeting hgcAB and sulphate-reducing bacteria (SRB) in samples collected throughout blooms. Together, our study sheds light on the cycling of mercury, microbial community composition, and water quality, thereby further guiding safe management and cleanup of decomposing algae on Canadian onshore beaches.

T831013

SUSTAINABLE NANOTECHNOLOGY: ALGAE-BASED SYNTHESIS OF COPPER OXIDE NANOPARTICLES. **Vaughn Mangal***; Reem Mahamoud. Brock University, Department of Chemistry (vmangal@brocku.ca).

Copper oxide nanoparticles (CuO NPs), are widely utilized in many disciplines of research, including biomedical and material sciences, leading to their increased demand for production. While conventional synthesis methods have demonstrated scalability and purity, the reality is that the use of harsh reducing agents in large quantities and high-energy inputs raises environmental and safety concerns. Addressing these concerns has driven researchers to adopt greener methods that use biological organisms, notably plant extracts that contain the necessary biomolecules to facilitate

NP formation under milder conditions. While recent advancements highlight terrestrial plants and lab-grown microbial cultures, other underexplored sources for NP formation may include a combined approach of bioremediation and sustainable nanoparticle synthesis. This study brings forth a new approach to resource recovery for environmental management practices of algal blooms, which repeatedly pollute our Great Lakes, but offer a viable underutilized source of biomolecules that can encapsulate Cu for nanoparticle formation. Nanoparticles were characterized using a combination of particle size analysis, x-ray diffraction (XRD), inductively coupled plasma mass spectrometry (ICP-MS), scanning electron microscopy with an electron dispersive x-ray (SEM-EDX), Fourier transform infrared spectroscopy (FTIR), and liquid chromatography quadrupole-time-of-flight mass spectrometry (LC-QTOF) techniques, to validate synthesis, characterize morphology, quantify copper and identify actively participating biomolecules. Preliminary findings highlight optimal harvesting windows and conditions of the algal biomass, which affect nanoparticle yield and stability. The utilization of algal blooms in sustainable nanoparticle research focuses on advancing circular economy strategies by converting pollutants into valuable nanomaterials.

T940718

NMR STRUCTURAL STUDIES IN THE NATIVE STATE – INSIGHTS TO MEMBRANE PROTEINS AND LIPID-BOUND PROTEINS. **Francesca M. Marassi***. Departments of Biophysics and Biochemistry, Medical College of Wisconsin, Milwaukee, WI 53226-3548, USA (fmarassi@mcw.edu).

The direct characterization of proteins in their native environment has long been a major goal and driver of technology development in all areas of structural biology. While structural biology has advanced significantly by working with purified proteins in crystalline, water-soluble, or lipid-reconstituted states, the importance of environmental effects on protein structure has been appreciated for some time, and in situ structural studies are particularly important for membrane proteins, which have coevolved with their lipidic membrane components for specialized inside-outside membrane functionalities. NMR is exceptionally well suited for in situ structural studies. Since its origin, NMR has continued to grow as a technology with broad applications in physics, chemistry, biology and medicine, its versatility stemming from its ability to provide atomic-level information for molecules in heterogeneous and complex environments, including living systems. Optimized protein expression strategies, isotope labeling schemes, powerful instrumentation and specialized pulse sequences offer new opportunities for exploring the growing and important area of in situ structural biology. Here, we will describe recent advances that enable NMR structure-activity studies of membrane proteins and lipid-associated proteins in situ.

T91031

CHEMICAL TRACE EVIDENCE: ANALYTICAL OPPORTUNITIES AND CHALLENGES. **Sanela Martic***. Department of Forensic Science, Environmental Life Sciences, Materials Science Program, Trent University, Peterborough, ON, Canada (sanelamartic@trentu.ca).

The chemical trace evidence plays critical role in forensic investigations. For example, glass, fiber, paint, fingerprints and gunshot residues are often found at crime scenes and their chemical analysis can provide key insights. Our discoveries in the field of chemical trace evidence will be discussed. We explored various analytical methods, such as ICP-MS, for analysis of gunshot residues on fabrics, focusing on transfer and persistence. New fluorescent materials were developed for latent fingerprint development allowing fluorescence spectroscopy to be used for imaging fingerprints on complex substrates. The utility of glass, fiber, and paint evidence was evaluated in the context of legal case proceedings across Canada.

T930512

DIVERSITY OF ELECTROCHEMISTRY. **Sanela Martic***. Department of Forensic Science, Environmental and Life Sciences Program, Trent University, Peterborough, Canada, K9L0G2 (sanelamartic@trentu.ca).

Electrochemistry is a powerful area of analytical chemistry with plenty of opportunities for new discoveries. Using proteins, we demonstrated that fundamental biomolecular interactions can be monitored and targeted. The electrochemical sensors were developed for detection of various analytes, from health through forensic to environmental applications. Even carbon-carbon bond formation and electrosynthesis have been achieved as an alternative to the traditional synthetic methods. Our newest research efforts in electrochemistry will be also described.

T81053

THE GOOD, THE BAD AND THE UGLY: A TALE OF MICROSCOPIC CORROSION. **Janine Mauzeroll***. Department of Chemistry, McGill University, 801 Sherbrooke St. West, Montréal, Québec H3A 0B8 (janine.mauzeroll@mcgill.ca).

Electrochemical materials react, evolve and degrade. Material activity is often tied to their inhomogeneities in the chemical, physical and mechanical properties. As such to understand, track, and inform the material design, in-situ spatial temporal microscopies are needed. This talk will focus on the good, the bad and the ugly of electrochemical microscopies. Specifically our efforts related to scanning electrochemical imaging microscopies applied to metal alloys but also recent work on carbene protection of metal alloys will be discussed. Specifically, we will discuss how variations in droplet wettability affect localized corrosion during scanning electrochemical cell microscopy (SECCM) on stainless steel. The droplet dynamics are influenced by stainless-steel microstructural features and surface conditions–such as surface roughness, inclusions, and the addition of an oil

layer. As opposed to previous work on aluminum alloys, droplet spreading is promoted by oil immersion, which leads to an increase in the cathodic currents. Rougher surfaces hinder droplet spreading, largely due to the droplet pinning effect, and exhibit higher pitting corrosion incidences compared to smoother surfaces. Moreover, the presence of inclusions intensifies pitting initiation and constrains the landing area (droplet size). We report that while the landing area does not affect the number of metastable pits, small landing areas lead to a high probability of stable pitting. We also demonstrate that this method may be applied to cracked and fatigued samples, where increase pitting probability occurs close to the crack area.

T91091

NON-TARGET ANALYSIS BY LIQUID CHROMATOGRAPHY–HIGH-RESOLUTION MASS SPECTROMETRY: APPLICATION IN ALGAL BIOTOXIN SURVEYS. **Elliott J. Wright***; Daniel G. Beach; Pearse McCarron. Metrology Research Centre, National Research Council of Canada, 1411 Oxford Street, Halifax, NS, B3H 3Z1, Canada (pearse.mccarron@nrc-cnrc.gc.ca).

Liquid chromatography–high-resolution mass spectrometry (LC–HRMS) enables provides potential for non-target analysis (NTA) of algal biotoxins, providing potential for comprehensive class chemical screening and retrospective analysisof environmental samples. In this work an LC–HRMS data acquisition methods and processing workflow s using metabolomics software were was developed to analyse samples for a broad range of marine and freshwater biotoxins that are produced by species of harmful algae classes, including known toxins and related analogues. The approach was utilized to provide novel insights on the profile, homogeneity and stability of A matrix biotoxin reference material containing multiple biotoxins was used to develop and verify the performance of the overall procedures, including a mussel matrix for marine biotoxins and a cyanobacterial matrix for cyanotoxins. Producing information on hundreds of toxins, NTA provided significant advantages over conventional targeted analysis. These efforts established and validated processes for analyzing environmental sample sets and tThe methods technique were was then applied to passive samplers deployed in Puget Sound,coastal areas of Washington State (USA), between 2016 and 2018, and to an archived sets of passive samplers deployed in Ship Harbour, Nova Scotia (Canada), between 2004 and 2006. Evaluation of the Puget SoundWashington State data set revealed varied trends in toxin profiles including dinophysistoxins, pectenotoxins, yessotoxins, cyclic imines and goniodomins. Similarly diverse toxin profiles were observed in the samplers from Ship HarbourNova Scotia sets, including analogues not reported in previous targeted analysisstudies. The NTA experiments provided detailed information on spatial and temporal distribution of toxins on in both the Northwestern and Northeastern coastal regions s of North America, which is valuable for managing risks presented by future research on harmful algae and toxins in the region. Overall, theThe work highlights best practices for use of NTA, and demonstrates a modern approach for comprehensive algal biotoxin analysissurveillance.

T840717

STRIKING DIFFERENCES IN INCLUSION BODY STRUCTURE AND STABILITY CONNECT TO NATIVE MONOMER PROPERTIES. **Elizabeth M Meiering***; Bruna Siebeneichler; Pedro Rodriguez Cruz; Xiaoyue Liu; Dalia Naser; Anna Schaefer. Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada (meiering@uwaterloo.ca).

Protein aggregation is central to aging, disease and biotechnology. While there has been recent progress in defining structural features of cellular protein aggregates, many aspects remain unclear. We have investigated inclusion body (IB) formation in E. coli using recombinant proteins spanning major structural classes: β-sheet (SOD1, Adnectins/monobodies), α-helix (apomyoglobin), and disordered low-complexity domains (TDP43-LCD, HnRNPA2-LCD). Disease-associated and designed variants are analyzed alongside wild-type counterparts and soluble precursor proteins. Combining quenched H/D exchange NMR, ATR-FTIR, proteolytic stability assays, and chemical denaturation, we uncover remarkable differences in IB architectures. SOD1 and Adnectins exhibit extensive backbone amide protection and high IB stability, contrasting sharply with TDP43/HnRNPA2-LCDs, which show minimal protected regions and low stability. Apomyoglobin constructs display intermediate characteristics. This striking structural heterogeneity reshapes the prevailing view of IBs as generally similar and amyloid-rich by revealing a continuum of conformations influenced by characteristics of the native monomer. The relationships between IB characteristics and predicted as well as observed protein aggregation in vitro and in vivo contribute to unravelling and ultimately controlling aggregation in protein engineering and in disease.

T830614

CHICKENS AND EGGS: SERS MONITORING OF GOLD NANOPARTICLE LIGAND EXCHANGE. **Vicki Meli***; Samuel A. Levesque; Anna L. Ritter; Nghi La; Cynthia J. McNair, Nathan M. Regular; Edith R. Mummery. Mount Allison University, Department of Chemistry and Biochemistry, Sackville NB E4L 1E4, Canada (vmeli@mta.ca).

Gold nanoparticles (AuNP) have attracted significant attention for applications in metamaterials, plasmonics, and surface enhanced Raman spectroscopy (SERS) due to their plasmonic properties and adjustable morphology. Control over the surface chemistry of AuNP plays an important role in the ability to design AuNP for their use in these, and other, applications. Many applications require a mixed ligand shell and a reliable means of preparation. At the same time, SERS offers several advantages as a characterization tool for routine AuNP ligand shell characterization but is not commonly employed for this purpose. Our recent efforts to track the ligand exchange on gold nanoparticles (spheres and rods) using SERS will be described. Emphasis will be placed upon the ligand exchange of cetyl trimethylammonium bromide (CTAB) for bifunctional alkyl thiol systems. Ligand exchange of CTAB for polyethylene glycol thiol (PEG-SH) will first be described with characterisation by SERS, ATR-FTIR, UV-vis-NIR, and zeta potential. Secondary ligand exchange taking place on the PEG-AuNR is monitored over time using mercaptoundecanoic acid as well as a

SERS-active thiol, p-terphenyl-4,4''-dithiol (TPD). Such ligand exchange monitoring using SERS applied to spherical gold nanoparticles will also be presented and compared with that of the nanorods.

P750142

PATHWAY STRENGTH: AN ALGORITHM THAT COMPUTES THE BIDIRECTIONAL STRENGTH OF METABOLIC PATHWAYS FROM STEADY STATE LIPIDOMIC MEASUREMENTS AND UTILIZATION AS A LIPID METABOLIC INDEX TO ASSESS NOVEL TRANSGLYCOSIDEASE FUNCTION IN GBA1-PD PATIENTS. **Steffany A.L. Bennett [1]; Zach Miller***[1]; Miroslava Cuperlovic-Culf [2]; Thao Nguyen-Tran [1]. [1] Neurolipidomics Lab, India Taylor Lipidomic Research Platform, Ottawa Institute of Systems Biology, Department of Chemistry and Biomolecular Sciences and Department of Biochemistry, Microbiology and Immunology, University of Ottawa; [2] Digital Technologies Research Centre, National Research Council of Canada, Canada, Ottawa, ON. (zmill071@uottawa.ca).

Lipidomic signatures in biofluids are under assessment as potential prognostic and monitoring biomarkers. The metabolic interpretation of these steady-state signatures is often challenging due to (1) the diversity and complexity of the lipidome, (2) the interconnection of lipid metabolism wherein the level of each lipid molecule is the result of multiple enzymatic reactions, and thus (3) statistical changes (or lack thereof) in lipid abundances is not simply a direct result of a mutation but rather a snapshot of a change of state across the entire metabolic system. We present here a strategy to derive a clinically relevant metabolic index of this change in state from steady-state lipidomics acquired using nanobore reversed-phase liquid chromatography-electrospray ionization-differential mobility spectrometry, tandem mass spectrometry (RPLC-ESI-DMS-MS/MS) followed by information-dependent-acquisition of enhanced product ion scan (IDA-EPI) in different matrices. This index was developed and validated in cell culture treated with enzymatic inhibitors and deployed in assessment of plasma samples from GBA1-Parkinson's patients. We report here our quantification of β-GlcCers and β-GalCers, as well as β-GlcChol and β-GalChol and show that the expression of GBA1-PD variants alters GBA1's transferase activity (a novel gain of GBA1 enzymatic function) in human plasma.

T740417

FROM DISCOVERY TO APPLICATION: ADVANCING SEAFOOD SAFETY THROUGH CIGUATOXIN RESEARCH. **Elizabeth M. Mudge ***[1]; Christopher O. Miles [1,2]; Alison Robertson [3]; Pearse McCarron [1]. [1] National Research Council of Canada, Biotoxin Metrology, Metrology Research Centre, 1411 Oxford St, Halifax, NS, B3H 2Z1, Canada; [2] Norwegian Veterinary Institute, Ås, Norway; [3] School of Marine & Environmental Sciences, University of South Alabama, Mobile, AL, USA. (elizabeth.mudge@nrc-cnrc.gc.ca).

Ciguatoxins (CTXs) are lipophilic ladder-framed polyethers that accumulate in fish tissues and cause ciguatera poisoning (CP). CP is the most prevalent marine biotoxin related seafood poisoning globally, disproportionately affecting residents of tropical and subtropical regions that rely on fish for sustenance. Reports of CP in non-endemic regions are growing due to increased travel and seafood importation, while changes in ocean temperatures are expanding the distribution of the toxin-producing microorganisms. CTX monitoring is hampered due to low toxicity thresholds (0.01–0.1 ng/g), the presence of various CTX analogues, complex sample extraction, matrix interferences, poor LC–MS ionization and a lack of reference materials. Recent research on Caribbean CTXs has enabled significant advances in analytical measurements, including the development of novel clean-up procedures [1], derivatization techniques [2] and extraction procedure optimization. The discovery of a previously unknown algal produced C-CTX precursor [3] facilitated the preparation of critically needed reference materials. This research lays the foundation for CTX monitoring programs that are essential for reducing incidences of ciguatera poisoning globally.

T930112

INTELLIGENT DIFFERENTIAL ION MOBILITY SPECTROMETRY (IDMS): A DEEP NEURAL NETWORK THAT PREDICTS OPTIMAL SPACE-RESOLVED ION MOBILITY PARAMETERS FOR ISOMERIC. **Thao Nguyen-Tran***[1;2]; Xun Xun Shi [1,2]; Graeme P. Taylor [1,2]; Mathieu Lavallée-Adam [2]; Theodore J. Perkins [2]; Steffany A. L. Bennett [1,2]. [1] Neurolipidomics Lab, India Taylor Lipidomic Research Platform, and Department of Chemistry and Biomolecular Sciences, University of Ottawa, Ottawa, ON, Canada K1N 6N5. [2] Ottawa Institute of Systems Biology, Department of Biochemistry, Microbiology and Immunology, University of Ottawa, Ottawa, ON, Canada K1H 8M5. (tnguy224@uottawa.ca).

DMS separates gas-phase ions based on their mobility difference in high versus low electric field (Separating voltage – SV). The trajectory of ions is corrected by a DC offset (Compensation voltage – CoV) and ions are redirected to the detector, such as the mass spectrometer (MS). We previously combined DMS and LC-ESI-MS/MS [1] as an analytical method to separate and quantify isomeric cerebrosides, β-glucosylceramides (GlcCers) and β-galactosylceramides (GalCer) in human biofluid. DMS method development is labour-intensive, and highly dependent on the availability of pure synthetic lipid standard for each isomer. Where synthetic standards do not exist, method development is not possible. We present here iDMS - a machine-learning expansion to current DMS capabilities by predicting the required combination of SV and CoV to separate a given pair of isomeric sphingolipid ions. iDMS was trained on two chemical features of a lipid: its hydrocarbon chain length and unit of unsaturation. iDMS neural network architecture was optimized using the 17 pairs of GlcCers and GalCers in [1]. Considering the performance and minimal number of empirical data required to make accurate prediction, iDMS accelerates LC-ESI-DMS-MS/MS method development and enhances its role in biomarker discovery.

P750940

THE FATE OF SILVER NANOPARTICLES IN ENVIRONMENTAL MATRICES. **Jessica Ni***; Zhe She. Queen's University, Department of Chemistry, 90 Bader Lane, Kingston, ON, K7L 3N6, Canada. Sarah Jane Payne, Queen's University, Department of Civil Engineering, Queen's University, 58 University Ave, Kingston, ON, K7L 3N6, Canada. (19jn32@queensu.ca).

Silver nanoparticles (AgNPs) are metallic colloids ranging from 1-100nm in size. Due to their antimicrobial activity, they are increasingly incorporated into a range of consumer products, leading to environmental contamination. There is limited knowledge on the fate and effects of AgNPs after release leading to health and environmental concerns. This study will evaluate the stability of AgNPs using a nanoparticle tracking analyzer (NTA), that can optically determine the hydrodynamic size, concentration in terms of particles/mL, and zeta potential of nanoparticles in solution. To establish a baseline understanding of AgNP behaviour, they will be introduced to a variety of matrices that mimic the conditions AgNPs may experience in the environment. ICPMS is a well-established method to quantify trace metal contaminants, providing concentrations in the µg/L range. However, with aggregation being a known pathway of AgNP combined with studies reporting size dependent antimicrobial effects1, this study will also compare how AgNPs with the same mass concentration, may potentially have different effects based on their particle count.

T81045

GC-MS PROFILING OF ORANGE PEEL EXTRACT AND ITS PROPERTIES IN DAIRY AND PLANT-BASED YOGHURT. **Oluwasayo Esther Ogunjinmi***[1]; Olayombo Margaret Banwo [1]; Basheet Tobiloba Fayoyin [2]; Anthony Feranmi Ogunsola [1]. [1] Department of Industrial Chemistry, Abiola Ajimobi Technical University, Ibadan, 200255, Nigeria; [2] Department of Physics and Science Laboratory Technology, Abiola Ajimobi Technical University, Ibadan, 200255, Nigeria (ogunjinmio@gmail.com).

The global rise in demand for functional foods has driven interest in the development of dairy- and plant-based products enriched with natural bioactive compounds. Citrus fruits produce a lot of byproducts after processing, which was regarded as waste. Bioactive compounds present in citrus peels are useful for the food industry and human health, with the potential to mitigate the risk of chronic illnesses and disorders. This study investigated dairy- and cashew-based yogurts enriched with orange peel extract (1%) and evaluated their antioxidant, cytotoxic, and sensory properties. Orange peel extract was obtained through maceration in ethanol, analysis of its phytochemical constituents using Gas Chromatography-Mass Spectrometry (GC-MS). The antioxidant activity was assessed with the 2,2-diphenylpicrylhydrazyl radical method, while cytotoxicity was evaluated using brine shrimp lethality assay, with all analyses done in triplicate. GC-MS revealed 27 compounds, with 9-Octadecenoic acid (Z)-methyl ester as the main component. Cashew-based yogurt enriched with orange peel extract demonstrated higher antioxidant (IC50 = 679.22±5.36 µg/mL) and cytotoxicity (LC50 = 309.44±0.00 µg/mL) compared to dairy-based yogurt (IC50 = 1213.14±1.55 µg/mL; LC50 = 701.17±0.00 µg/mL). Sensory evaluation showed similar taste and texture, but significant differences

in colour and appearance. Fortified cashew-based yogurt exhibited notable therapeutic properties and fair consumer preference.

T840116

AN AMBIENT IONIZATION PLATFORM FOR THE ANALYSIS OF ADHERENT CELL CULTURES AND FFPE TISSUE SAMPLES. **Richard Oleschuk***[1]; Mina Alidoust [1]; Rachel Wood [1,2]; Malek Hassan [1]; Bryan Young [1]; Jess Deng [1]; Randy Ellis [3]; Chris Nicol [2,4]. [1] Department of Chemistry, Queen's University, Kingston, Ontario, Canada; [2] Departments of Pathology and Molecular Medicine, Queen's University, Kingston, Ontario, Canada; [3] School of Computing, Queen's University, Kingston, Kingston, Ontario, Canada; [4] Sinclair Cancer Research Institute, Queen's University, Kingston, Ontario, Canada (oleschuk@queensu.ca).

Ambient ionization mass spectrometry (AI-MS) has significantly advanced analytical workflows by enabling direct chemical interrogation of samples with minimal or no preparation. Our laboratory is focused on further democratizing mass spectrometry through the development of a robust, automated liquid microjunction surface sampling probe (LMJ-SSP) platform capable of reproducible, high-throughput analysis across diverse biological matrices. This system integrates automated optical sample recognition for region-of-interest targeting, in-line deparaffinization for formalin-fixed paraffin-embedded (FFPE) tissues, and precision positional control to ensure consistent microjunction formation and solvent-surface interaction. Real-time feedback sensing enables dynamic optimization of sampling conditions, improving extraction efficiency and signal stability. Coupled with high-resolution mass spectrometry, the platform supports rapid, spatially resolved profiling of metabolites, lipids, and small molecules from both adherent cell cultures (e.g., human breast cancer and clear cell renal cell carcinoma lines) and tissue specimens, including fresh frozen and FFPE melanoma samples. Advanced data processing pipelines incorporating multivariate statistical analysis and machine learning facilitate robust tissue classification. By unifying automated sampling, ambient ionization, and data-driven analysis, the LMJ-SSP based platform enables rapid (<minutes per sample), reproducible chemical characterization. The LMJ-SSP approach represents a significant step toward real-time, accessible chemical analysis for complex and demanding sample types.

T82085

ISOTOPE DILUTION CALIBRATION CURVE FOR INORGANIC ANALYSIS AND METAL SPECIATION: THE CASES OF LEAD AND METHYLMERCURY. **Enea Pagliano***. Metrology Research Center, National Research Council Canada, 1200 Montreal Road, Ottawa,Ontario, K1A 0R6, Canada (enea.pagliano@nrc-cnrc.gc.ca).

Isotope Dilution Mass Spectrometry (IDMS) is a high-precision quantitation method frequently used for inorganic analysis and metal speciation. Traditionally, IDMS is implemented using complex model equations directly applied without any visual support of the calibration process. This approach deviates from common practices in instrumental analytical chemistry, where the use of calibration curves remains prevalent. For this reason, the IDMS method was revised to include a graphical-based calibration. The graphical IDMS generates calibration curves by fitting the data with a nonlinear rational function of the following form: $y = (ax + b) / (1 + cx)$ and provides results by interpolation. The novel approach maintains the same level of metrological rigor as the traditional formulation, but it is simpler to implement. IDMS calibration curves can be visually inspected, used for high-throughput analysis over a wider range, and account for isotopic mismatching between standards and samples. In this talk, the graphical IDMS is described from its first principles and implemented for high-precision determination of lead and methylmercury in the NRC DORM-5, KRIK-1, and ROCA-1 Certified Reference Materials for food safety

T82095

IDENTIFICATION AND VERIFICATION OF POTENTIAL PER- AND POLYFLUOROALKYL SUBSTANCES (PFAS) IMPACTED GROUNDWATER. **Adrian Pang***[1]; Dylan Roberts [2]; Dean Morrow [1]; Taylor Vereecken [1]; Iris Koch [1]; Kela Weber [1]. Military College of Canada, Department of Chemistry and Chemical Engineering, 12 Verité Ave, 17000 Station Forces, Kingston, ON K7K 7B4, Canada. 2Greenstone Engineering Ltd, 8A Cumberland Street North, Suite #203, Thunder Bay, ON P7A 4K9 (adrian.pang2@rmc-cmr.ca).

Per- and polyfluoroalkyl substances (PFAS) are large class of anthropogenic and recalcitrant chemicals that are primarily categorized using their carbon fluorine bonds. Containing a hydrophobic tail and hydrophilic functional head, PFAS usage has become ubiquitous across several industrial sectors. Despite the documented use of PFAS in these sectors, not much is known about the number of potential facilities that may act as a point source release of PFAS into the environment. The purpose of this project was to estimate the number of potential PFAS point sources and to validate some of the identified sites via groundwater samples within and/or adjacent to the site. The approach to reliably estimate the number of sites will be discussed, along with the occurrence of PFAS found at some of the identified sites. Using target and non target approaches on a liquid chromatography high resolution mass spectrometry, results from the analysis show that PFAS concentration and composition varied across sites and industrial sectors. However, short chain perfluorocarboxylic acids (PFCA) were found to be ubiquitous in all sites. The focus will be on ultra-short chain PFAS compounds that exhibit low hydrophobicity that are not routinely measured.

T81081

MERCURY SPECIATION IN WHOLE BLOOD USING LIQUID CHROMATOGRAPHY WITH VAPOR GENERATION COUPLED TO ICP-MS: FITNESS FOR PUBLIC HEALTH PURPOSES. **Emily J. Pacer***[1]; Christopher D. Palmer and Patrick J. Parsons [2]. [1] Division of Environmental Health Sciences, Wadsworth Center, NY State Department of Health, Albany, NY 12237; and Department of Environmental Health Sciences, University at Albany, Rensselaer, NY 12114 (Patrick.Parsons@health.ny.gov).

Speciation analysis is critical for a complete assessment of human exposure to (Hg). Typically, urine is used to assess inorganic Hg, (iHg) exposure, and whole blood is used to assess both methylmercury, MeHg, and/or iHg exposures. We developed a new speciation method using Liquid chromatography (LC) to separate iHg from MeHg species in whole blood with isocratic elution on a C8 column and detection using ICP-MS/MS [1]. We used vapor generation (VG) post-column to boost the Hg signal-to-noise ratio and thereby obtain lower limits of detection (LODs) for both iHg and MeHg. If ethylmercury (EtHg) is present in the blood sample, (e.g., NIST SRM 955c), then this can be captured by simply extending the LC elution time from 4 to 8 minutes. The method was validated against NIST SRM 955c Toxic Metals in Caprine Blood and NIST SRM 955d Toxic Elements and Metabolites in Frozen Human Blood. Archived blood materials from External Quality Assessment schemes, and blood-based quality control materials from the CDC were analyzed to provide additional method characterization data. The method was used to analyze archived human blood samples from 12 NY City residents, who had used Hg-containing skin lightening creams.

P750734

PROTEINS UNDER PRESSURE: INVESTIGATING STABLE INTERMEDIATES OF THE PYRIFORM SPIDER SILK REPETITIVE DOMAIN. **Charlotte Polo***. Dalhousie University,Department of Biochemistry & Molecular Biology, Halifax, NS, Canada. (charlotte.polo@dal.ca).

A female orb-weaving spider can produce seven different silks, each with distinct properties suited to its function. Despite advances in the study of spider silks, most research on spider silk protein (spidroin) self-assembly has focused on dragline silk. The lesser characterised silk, pyriform silk, is used by spiders to anchor webs. The spidroin component of this silk, PySp1, from Argiope argentata contains a repetitive domain with 234-residue repeat units comprising α- helical domains connected by disordered linkers; However, in the fibrous state, PySp1 has been found to have substantial β-sheet content. We previously engineered a truncated PySp1 repeat unit (Δ1-62+Δ198-234-HPy1) that maintains the α-helical structuring and fold. We aim to elucidate the mechanism of structural rearrangement within the PySp1 repeat unit by probing for intermediate states of Δ1-62+Δ198-234-HPy1. We hypothesize that through stabilizing conformations of lower partial molar volume, high pressure nuclear magnetic resonance spectroscopy will allow observation of such states, likely corresponding to intermediates in self assembly. Δ1-62+Δ198-234-HPy1 responds distinctly to pressure versus chemical and thermal perturbation, deviating from the expected two-state

unfolding process, suggesting the possibility of visualizing intermediate states using pressure. This research is broadening the understanding of spidroin self-assembly, allowing for the optimization of various engineered spidroin-based materials.

P750122

DIFFERENTIATION BETWEEN CITRULLINATION AND DEAMIDATION USING PEPTIDE RETENTION PROPERTIES IN 2D LC-MS/MS. **Alexandre Prefontaine***; Rene Zahedi; Oleg Krokhin. University of Manitoba, Department of Biochemistry and Medical Genetics, 745 Bannatyne Avenue, Winnipeg, MB R3E 3P4, Canada; University of Manitoba, Department of Internal Medicine, 820 Sherbrook Street, Winnipeg, MB R3A 1R9 (prefont5@myumanitoba.ca).

Citrullination is a clinically relevant post-translational modification associated with many human diseases1. Mass shift of +0.984Da, identical to deamidation makes differentiation between these two modifications by mass spectrometry difficult. The chromatographic properties of modified peptides provide an orthogonal means of identification. To acquire abundant sample data for training of sequence-specific retention models, human Jurkat Lys-C digests were citrullinated in vitro using peptidylarginine deaminase 2. Retention properties were reported in hydrophobicity index (HI, % ACN) using a calibration mixture of standard peptides 2. The 2D LC-MS/MS acquisitions resulted in confident identification of ~5000 and ~20000 pairs of modified – non-modified peptides for deamidation and citrullination, respectively – the largest assembly of citrullinated peptides ever reported. Seven different separation modes were tested to determine which 2DLC pairing should be chosen. The most promising separation chemistries were determined by calculating the mean retention difference between citrullination and deamidation (ΔΔHI), the separation between both populations of modified peptides (Cohen's d), and the probability of differentiation without training from the area under the curve (AUC). The final pipeline and classification algorithm integrates sequence-specific classification in both dimensions.

T830314

FROM ADULTS TO CHILDREN: A COMPARATIVE STUDY OF ETV-ICPOES AND ETV-ICPMS FOR HAIR-BASED SEX DETERMINATION. **Darrian Prendergast***; Ella Lapointe; Diane Beauchemin. Queen's University, Department of Chemistry, Kingston, ON K7L 3N6, Canada (18ddap@queensu.ca).

Determining the sex of children's remains is constrained by the limited number of available techniques, many of which are poorly established, controversial, or primarily applied to adults. Previous work used electrothermal vaporization (ETV) for direct solid analysis by inductively coupled plasma optical (ICP) emission spectrometry (OES) to deduce the sex of adults [1] and mummies [2]. The higher sensitivity of ICP mass spectrometry (MS) could also be useful for investigating subtle compositional differences in human hair. This presentation will first outline ETV-ICPOES

advancements on this project to date, followed by preliminary results obtained by ETV-ICPMS for the first time. All head hair samples were washed with doubly deionized water, dried, and ground into a fine powder. Data were processed according to the analytical technique used. This was followed by multivariate statistical analysis using Minitab software. Principal component analysis and linear discriminant analysis were applied as dimensionality reduction techniques to identify elements that act as key differentiators of sex. These results contribute to the development of an improved method for sex determination of adult and children's remains.

T91071

LEVERAGING ALLOSTERY IN SMALL MOLECULE AND PROTEIN DRUG DISCOVERY - NEW INSIGHTS USING NMR. **R. Scott Prosser***. [1] Department of Chemistry, University of Toronto, Chemical and Physical Sciences, University of Toronto at Mississauga, Mississauga, ON L5L 1C6, Canada; [2] Department of Biochemistry, University of Toronto. Medical Science Building, Toronto, ON M5S 1A8, Canad (scott.prosser@utoronto.ca).

Modern drug discovery is powered by large virtual screens and billion-compound docking campaigns, which have become increasingly powerful through the lens of Artificial Intelligence (AI). Hits from such approaches may then be funnelled through high-throughput techniques such as affinity selection mass spectrometry (ASMS) or DNA-encoded chemical libraries. We have addressed several critical bottlenecks associated with the discovery process with a focus on allosteric small molecule and therapeutic discovery in the case of GPCR targets. Targets are first evaluated computationally to identify allosteric interfaces and networks. Fragments or nanobodies are then screened to bind to these putative allosteric hotspots in the presence of saturating concentrations of ligands which simultaneously stabilize the desired activation state. Our libraries consist of non-flat, sp3-hybridized fluorinated molecules with distinct nucleophiles that can be readily conjugated. The position-sensitive electrophiles at chiral sites on these scaffolds allow us to generate a vast library of small molecules which are not currently commercially available. Our synthetic procedures rely on established protocols to conjugate commercially available chemotypes to our scaffolds. Using Affinity Selection Mass Spectrometry ASMS and 19F NMR CPMG-filtered spectroscopy, we have identified small molecule adjuvants that bind to putative allosteric sites. Cell assays confirm their pharmacological effects. In all studies, NMR of the target provides a readout of the functional ensemble (active, inactive, and intermediate states) and thus, a mechanistic understanding of response. Using minimal labeling that is amenable to E. coli, yeast, and insect cell systems, we can efficiently and inexpensively enrich media with 13C-methyl-tryptophan (Trp) or tag the target with next generation 19F NMR reporters that are ultra sensitive to microenvironment. Structure Activity Relations are discussed in the context of response to allosteric drugs.

T82086

AUTOMATED AND SIMULTANEOUS LC COUPLED WITH -ICPMS AND -QTOF-MS. **C Derrick Quarles Jr***[1]; Patrick Sullivan [1]; Brianna Dufek [1]; Daniel Dobson [2]; Mathis Athmer [3]; Uwe Karst. [1] Elemental Scientific, Inc., Omaha, NE, USA; [2] Genentech, San Francisco, CA, USA. [3] University of Münster, Münster, Germany (Derrick.Quarles@icpms.com).

Elemental speciation is a well-known technique for determining the actual nature (species) of a given compound that may be present in environmental, biological, food, or pharmaceutical based samples. The nature of the given species can help determine if the compound is toxic or non-toxic and for organic synthesis it can help understand how efficient a synthetic process may be. Liquid chromatography-inductively coupled plasma mass spectrometry (LC-ICPMS) is the go-to method for determining the elemental species, whereas LC-MS is the go-to method for determining organic compounds/structures. Typically, these methods are run independently and require different chromatographic separation methods that are compatible with the ionization source (ICP or ESI). Here we present an automated method for simultaneous detection of elemental and organic compounds via split stream into an ICPMS and QTOF-MS. To demonstrate the capabilities two different applications were investigated: 1) Pd catalyst used in organic synthesis and 2) polyphosphonates and their transformation products in environmental samples.

T841018

HIGH-THROUGHPUT METHOD FOR ELEMENTAL AND ISOTOPIC CHARACTERIZATION OF NANOPARTICLES VIA SINGLE PARTICLE-ICP-TOF-MS AND SINGLE PARTICLE-MC-ICPMS. **C. Derrick Quarles Jr***[1]; Benjamin T Manard [2]; Hunter B Andrews [2]; Patrick Sullivan [1]. [1] Elemental Scientific, Inc., Omaha, NE, USA; [2] Oak Ridge National Laboratory, Oak Ridge, TN, USA. (derrick.quarles@icpms.com).

Single particle-inductively coupled plasma mass spectrometry (sp-ICPMS) has become an intriguing technique for understanding the chemical and isotopic nature of nanoparticles. These nanoparticles have an impact in the food industry, environmental implications, and may pose toxic threats to biological life forms. Here we present an automated, high-throughput method for the analysis of nanoparticles using a dedicated sample introduction system designed for single particle and single cell type applications coupled with an ICP-TOF-MS or a MC-ICPMS. Validation and performance metrics were determined for three different nanoparticles (50 nm Au, 100 nm Au, and 60 nm Ag/Au core shells). Following this validation, this method was implemented to investigate how well Pt is bound to protein functionalized magnetic microparticles via sp-ICP-TOF-MS. In addition, Nd based nanoparticles were analyzed using the newest generation of MC-ICPMS and compared with the previously developed metho on an ICP-TOF-MS.

P750733

APPLYING NMR SPECTROSCOPY TO EVALUATE SPIDER SILK PROTEIN STRUCTURAL CONVERGENCE AND PLASTICITY. **Jeffrey R. Simmons***[1]; Charlotte Polo [2]; Ivan Hung [3]; Frédérick Mentink-Vigier [3]; Jan K. Rainey [1,2,4]. [1] Department of Biochemistry and Molecular Biology, Dalhousie University, Halifax NS B3H 4R2, Canada. [2] Department of Chemistry, Dalhousie University, Halifax NS B3H 4R2, Canada. [3] National High Magnetic Field Laboratory (NHMFL), Tallahassee FL 32310, USA. [4] School of Biomedical Engineering, Dalhousie University, Halifax NS B3H 4R2, Canada (jan.rainey@dal.ca).

Spider silks are biomaterials produced and used for diverse applications, with mechanics comparable to Kevlar and high strength steel. Orb-weaving spiders produce up to seven distinct types of silk, six of which are fibrillar. Pyriform silk fibres are coated with a glue-like substance to form discs attaching silks together and anchoring spider webs to diverse substrates. We have engineered recombinant pyriform silk proteins based on a 234-amino acid (aa) unit repeated 21 times in the Argiope argentata central repetitive domain. Using triple-resonance solution-state NMR spectroscopy, we found that the solution-state structure of this protein contains an ordered 5 helix bundle, bridged by a sixth helix, flanked by long intrinsically disordered linkers at each end. The structure and architecture are modular, being retained upon addition of a second 234-aa repetitive unit, and resembles other evolutionarily distinct silk proteins despite a lack of sequence similarity. While the solution state structure is devoid of β-sheets, magic angle spinning (MAS) solid-state NMR demonstrates that recombinant silk fibers have a partial α-to-β transition. NMR spectroscopy therefore allow tracking of the pyriform silk structural transition from its soluble storage state to the fibrous state, providing fundamental insight into this intriguing material and enabling rational protein engineering.

P750735

STRUCTURAL CHARACTERIZATION OF THE REPEAT UNIT OF MESOTHELAE SPIDER SILK. **Suad Rashid***[1]; Noelle Aldous [1]; Jan K. Rainey [1,2,3]. [1] Department of Biochemistry & Molecular Biology, Dalhousie University, Halifax, Nova Scotia, B3H 4R2, Canada, [2] Department of Chemistry, Dalhousie University, Halifax, Nova Scotia, B3H 4R2, Canada, [3] School of Biomedical Engineering, Dalhousie University, Halifax, Nova Scotia, B3H 4R2, Canada. (suad.rashid@dal.ca).

Mesothelae spiders represent the most ancient lineage within the order Araneae, retaining ancestral features over millions of years. Unlike the evolutionary derived and widely studied orb-weaving spiders, which produce up to seven task-specific silks, mesothelae spiders produce a single, unspecialized silk fibroin that serve multiple purposes. Spidroin, the structural protein of spider silk, consists of conserved N- and C-terminal domains that mediate protein assembly and fiber formation and a variable central repeat domain that largely determines fiber mechanical properties. Structural characterization of the repeat domain is therefore critical for understanding silk mechanical performance and guiding the rational design of high-performance silk-based biomaterials. This work

aims to investigate the structure of the spidroin repeat unit of the mesothelae spider Liphistius malayanus. The gene encoding the repeat unit was synthesized, expressed in E. coli, and purified for structural characterization. Circular dichroism spectroscopy indicates that the repeat unit adopts a predominantly α-helical conformation, and 1H–15N HSQC NMR spectra show that the protein is well-folded in solution. Ongoing work is focused on structural evaluation using both solution-state and solid-state NMR, which will enable direct comparison with repeat units from other silks and provide insights into the molecular basis of silk performance and evolution.

T731015

COMPARISON OF CELLULAR IMMUNOLABELLING BETWEEN DEXTRAN-FUNCTIONALIZED QUANTUM DOTS (QDS), SUPRA-QD ASSEMBLIES, AND SUPER-QD ASSEMBLIES. **Kelly Rees***; Ghinwa H. Darwish; Agnes Szwarczewski; Jad Kaj, W. Russ Algar. Department of Chemistry, University of British Columbia, Vancouver, British Columbia, V6T 1Z1, Canada. (krees@chem.ubc.ca).

Cellular immunolabelling with dye-labelled antibodies is an important technique in bioanalysis and imaging; however, there is a need for brighter fluorescent probes in some applications. We have established a series of dextran-functionalized nanoparticles based on semiconductor quantum dots (QDs). These materials include individual dextran-coated QDs (Dex-QDs) [1] and both supra and super-nanoparticle assemblies of QDs (supra-QDs [2] and super-QDs [3]), which are 1–2 orders of magnitude brighter than Dex-QDs but are larger in size. We have previously demonstrated that all these materials can be used for extracellular immunolabelling using tetrameric antibody complexes (TACs), but we have not compared them concurrently. Here, we present a head-to-head-to-head comparison between Dex-QDs, supra-QDs, and super-QDs for cellular immunolabelling, and between the use of TACs and the covalent conjugation of antibodies. Physical characterization data and ensemble and single-particle fluorescence characterization for the materials are also presented. The immunolabelling trends are evaluated and compared to the material characterization data to determine the optimal material and immunolabelling strategy.

T830113

INTRODUCING MC-MICAP-MS: ADVANCING METAL ISOTOPIC ANALYSIS WITH NITROGEN PLASMA. **Anika Retzmann***[1]; Hadassah Michelle Dubois Recinos [1]; Gabriella Gelinas [1]; Kerri Miller [2]; Ashok Menon [3]; Michael Wieser [1]. [1] University of Calgary – Department of Physics and Astronomy, 2500 University Dr. NW, Calgary, AB T2N 1N4, Canada; [2] University of Calgary – Arnie Charbonneau Cancer Institute, 3280 Hospital Dr. NW,Calgary, AB T2N 4Z6, Canada; [3] Radom Instruments LLC, N27W23676 Paul Rd, Pewaukee, WI 53072, USA (anika.retzmann@ucalgary.ca).

Stable metal isotope ratios are a powerful tracer in (bio-)archaeology, geochemistry, materials research, environmental sciences, life sciences, and biomedicine. However, in conventional multi-collector inductively coupled plasma mass spectrometry (MC-ICP-MS), Ar-based spectral interferences generated by the Ar plasma restrict analytical performance for several elements, particularly at low mass resolution. This study presents the integration of a microwave inductively coupled atmospheric-pressure plasma (MICAP) ion source sustaining an N2 plasma with a multi-collector mass spectrometer, forming the novel MC-MICAP-MS platform for high-precision metal isotopic analysis. Replacing the conventional Ar plasma with a N2 plasma effectively eliminates Ar based spectral interferences. Analytical performance was evaluated for Sr, Ca, and Fe isotopes. The 87Sr/86Sr ratio achieved an internal precision of ≈0.007% (2SD) and an external repeatability of ≈0.010% (2SD), comparable to conventional MC-ICP-MS. Direct low-resolution measurements of Ca and Fe isotopes were possible due to the absence of Ar-based interferences. Oxide and doubly charged ion formation remained low under dry plasma conditions, and matrix elements such as Na and Mg showed negligible effects at 1:1 matrix-to-analyte ratios. Results for reference materials agreed with established values, demonstrating accuracy and robustness.

T940117

1H NMR ANALYSIS OF PETASE PRODUCT DISTRIBUTION AND SUBSTRATE SPECIFICITY REVEALS MECHANISTIC FEATURES OF PET HYDROLYSIS. **Constadina Rogers***; Amelia Wojtyk; David Langelaan. Dalhousie University, Department of Biochemistry & Molecular Biology, 5850 College Street, Halifax, NS B3H 4R2, Canada (dina.rogers@dal.ca).

Excessive polyethylene terephthalate (PET) plastic waste has negative impacts on the environment. Recent research on the engineering of PETase look to create an enzymatic recycling system as an environmentally friendly alternative to mechanical recycling. PETase catalyzes hydrolysis of PET producing major product mono-2-hydroxyethyl terephthalate (MHET) and minor products bis-2-hydroxyethyl terephthalate (BHET), terephthalic acid (TPA), and ethylene glycol (EG). PET can only be repolymerized from TPA and EG; thus, much research looks to create a system that yields majority TPA and EG rather than MHET. While there have been advancements in PETase engineering and identification of potential new PETases, the complexities of the PET reaction given its interfacial nature have been neglected. Here we demonstrate that PETase concentration can shift the distribution of PET hydrolysis products from majority MHET to majority TPA through product detection by 1H NMR. Additionally, we use pseudo-2D NMR to characterize the substrate specificity of PETase clarifying that it does possess weak MHETase activity; although, it was previously proposed not to. Combining these mechanistic findings together, we propose a newly modified model of PET degradation by PETase that is useful for future development of biological recycling processes.

T81043

A CUT ABOVE THE REST: ELEMENTAL FINGERPRINTING OF GRASS-FED AND GRAIN-FED ALBERTA BEEF FOR AUTHENTICATION AND RISK ASSESSMENT USING ICP-MS. **Alisa Gincher***; Angelo Trinidad; Nausheen Sadiq. Mount Royal University, Department of Chemistry, 4825 Mount Royal Gate SW, Calgary, AB T3E 6K6, Canada (nsadiq@mtroyal.ca).

A growing consumer focus on health, environmental sustainability, and food transparency has contributed to the expansion and success of the grass-fed beef market. Analytical chemistry has long played a critical role in food authentication and in assessing food safety at the elemental level. This study investigates differences in the elemental composition of store-bought grass-fed and grain-fed Alberta beef. Elemental analysis was conducted using an Agilent 7850 ICP-MS as an alternative to DNA-based authentication methods, which can be limited by DNA degradation. The quantification of Cd, Co, Cr, Cu, Fe, Mo, Mn, Ni, Pb, Se, and Zn enabled both authentication and food safety assessment of striploin and liver samples obtained from a local grocery store in Calgary, Alberta. Among these elements, Fe, Mo, Zn, and Cu were key discriminators between feed types. The effects of cooking on elemental composition were also evaluated. A radar plot was employed to generate visual "fingerprints," successfully distinguishing the elemental profiles associated with each diet. Notably, elevated lead concentrations were detected in all samples (2.47–2.76 mg/kg), exceeding the regulatory limit of 0.1 mg/kg by approximately 25-fold.

T81094

A DUSTURBING REALITY: EXAMINING ELEMENTAL DISSOLUTION AND HUMAN HEALTH RISK IN THE ATMOSPHERIC AGING OF DUST AND COAL FLY ASH USING ICP-MS. **Nausheen Sadiq***[1]; Catharina Veldman [1]; Madison Smith [1]; Arden Oglivie [1]; Wisam Mohammed [2]; Yara Khalaf [2]; Hind A. Al-Abadleh [2]. [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 (nsadiq@mtroyal.ca).

Iron (Fe) is a key element in atmospheric aging studies of particulate matter.[1] Understanding the chemical evolution of dust and coal fly ash is critical for assessing air quality, climate interactions, and human health impacts.2 This study investigates atmospheric aging in dust and coal fly ash samples from the USA, India, and Europe under acidic and organic conditions to simulate surface-catalyzed reactions To evaluate human exposure, artificial lung fluids were optimized to assess the bioaccessibility of ultrafine particles following realistic exposure times and microwave-assisted extraction. Multi-elemental analysis was performed using an Agilent 7850 ICP-MS. Elements of interest included Al, As, Fe, Cu, Mn, Pb, V, Zn, and Ni at varying pH. Results expand beyond previous Fe-focused work by incorporating multiple elements and extended time points (up to 14 days) to develop kinetic models of dissolution. Variations in fluid composition significantly influenced extraction efficiency and elemental release. This combined approach improves understanding of particle aging, elemental mobility, and potential health risks associated with inhalation exposure.

T830312

SWEAT, SPIT, AND SCIENCE: 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; Nausheen Sadiq. Mount Royal University, Department of Chemistry and Physics, 4825 Mount Royal Gate, Calgary, AB T3E 6K6, Canada (nsadiq@mtroyal.ca).

In a room full of evidence, is any of it truly reliable? For decades, analytical tools have been used to analyze forensic evidence.1 Previous studies have used hair to determine sex and ethnicity, demonstrating the utility of ICP in forensic research.1 This study investigates trace metal analysis of sweat and saliva as a viable tool for human identification. ICP-MS was used to analyze elemental profiles in sweat and saliva, with multivariate statistics applied to determine sex, ethnicity, and age. Sample size was increased (n = 100) to improve robustness. Classification accuracy varied by biofluid: sweat performed better for sex determination, while saliva showed higher accuracy for ethnicity, with comparable performance for age. Notably, age has not previously been evaluated in this context. In test sets, model accuracy exceeded random classification by 20%-90%. This study focuses on improving past results by increasing sample size, optimizing sample collection, and assessing sample stability. Finally, the impact of physical fitness will be tested on future participants by collecting data from individuals from a broad background of physical activity to see the impact lifestyle can have on elemental fingerprinting.

T930613

MECHANISTIC INSIGHTS TO PD-BASED THIN FILM HYDROGEN SENSING. **Julia E. Schmitt***; Michael S.Department of Chemistry, Dalhousie University, Halifax, NS, Canada (JSchmitt@dal.ca).

Hydrogen detection is essential for safety and process monitoring in energy, transportation and industrial systems, where early leak detection can prevent reaching flammability limits. Palladium (Pd)-based sensors traditionally operate through palladium hydride (PdH) formation, yet many studies evaluate performance in inert atmospheres and overlook the influence of oxygen under more realistic conditions.1In this work, hydrogen sensing in Pd thin films is investigated in the presence of 20% oxygen in nitrogen (synthetic air), to explore surface oxidation and oxide reduction. It will be shown that the dominant sensing mechanism depends strongly on the Pd nanostructure surface state and gas composition. In inert atmospheres and a reduced Pd surface oxide, sensing proceeds primarily through resistive PdH formation. In nitrogen or synthetic air with surface oxide, the response is governed by hydrogen-induced oxide reduction. At elevated temperatures or high hydrogen concentrations, hydride-dominated behavior is suppressed and catalytic hydrogen oxidation via water formation becomes significant. This presentation will explore our mechanistic

understanding of the competition between processes in Pd-based hydrogen sensing for real-world applications.

T740518

CREATING ADVANCED ANALYTICAL TOOLS USING ELECTROCHEMISTRY, SURFACE CHEMISTRY, AND 3D PRINTING. **Zhe She***. Department of Chemistry, Queen's University, 90 Bader Lane, Kingston, ON, Canada K7L 3N6. (zhe.she@queensu.ca).

There is a strong trend in developing portable chemical and biochemical detection methods to enable rapid, on-site, and low-cost detection. The development requires consideration of many factors, ranging from sensitivity and scope of detection to the stability of sensing devices and compatibility with real-time applications. We are interested in developing electrochemical sensors using the surface chemistry of molecules and materials for bacterial detection in environmental samples and heavy metal monitoring in drinking water. To complement this development, we have been exploring 3D thermoplastic printers as a cost-eUective approach. In this presentation, I will share our recent development of analytical tools and the challenges we have been facing.

P750736

ADVANCES TOWARD FULL-LENGTH STRUCTURAL CHARACTERIZATION OF VITRONECTIN, A MAJOR MULTIFUNCTIONAL SERUM PROTEIN. **Kyungsoo Shin***[1]; Rana Mansour; Karthika Samimuthu; Francesca M Marassi. Medical College of Wisconsin, Department of Biophysics, 8701 W Watertown Plank Rd, Milwaukee, WI 53226 (kshin@mcw.edu).

Vitronectin (Vn) is a ~75 kDa multifunctional glycoprotein implicated in diverse physiological and pathological processes, including bacterial pathogenesis and age-related mineralization disorders. Despite its importance as a therapeutic target, complete structural characterization has remained elusive due to its size, flexibility, and domain complexity. Vn is proposed to comprise a small N-terminal somatomedin B domain connected via a flexible linker to a large C-terminal hemopexin-like (HX) domain, which adopts a four-bladed β-propeller architecture with a helix-turn-helix motif and an extended flexible loop implicated in ligand interactions. Here, we report significant advances in defining the structure of full-length Vn, including its native post-translational modifications, enabled by recombinant production in a mammalian expression system. We demonstrate that the HX domain of Vn can be isolated by proteolytic digestion and confirmed by mass spectrometry. Furthermore, previously assigned NMR resonances corresponding to the β-propeller core are observed in the proteolytically derived HX domain, supporting the proposed structural model. Taken together, these findings provide new insights into Vn architecture and offer a foundation for interrogating its interactions with biomolecular and mineral partners involved in disease pathogenesis, with implications for guiding therapeutic development.

T840618

QUANTUM DOTS ENGINEERING: FROM FUNDAMENTAL TO PRODUCT DEVELOPMENT. **Gurpreet S. Selopala***; Swedha Madhua; Joshita P. Kumara; Msughter Guusua; Umair Sohaila; Sukhjinder Singha; Manmeet Kaur Chhinaa. Sustainable Nanoengineering Lab, Department of Engineering, Faculty of Agriculture, Dalhousie University, 39 Cox Rd, Banting Building, B2N 5E3, Truro, NS, Canada Corresponding author: Gurpreet S. Selopal (gs.selopal@dal.ca).

As the world moves towards a sustainable future, advanced materials engineering plays a key role in revolutionizing clean energy and smart agriculture. In this context, colloidal quantum dots (QDs) are widely used as building blocks for clean energy and smart agriculture technologies due to their size-, shape-, and composition-controlled optoelectronic properties arising from the "quantum confinement" effect. In particular, tunable broad light absorption range (300-2000 nm), large absorption cross-section, the possibility of multiple exciton generation (MEG) and hot-electron extraction before thermalization are key to building high-performing clean energy and their integration into smart agriculture technologies (i.e., greenhouse, sensors, etc.), opens new frontiers for precision farming and resource management. However, the performance of QD-based clean energy and smart agriculture devices remains lower than the expected theoretical value, primarily due to slow charge injection/transfer from QDs to scavengers and fast non-radiative carrier recombination within QDs and at the QDs/metal oxide/electrolyte interface. To address these challenges, surface engineering of QDs, in which the QD core surface is passivated by a shell layer of varying thicknesses and compositions, is an effective approach. This talk will cover the journey of colloidal QDs from fundamental research to practical product development. A detailed discussion of the impact of advanced surface engineering of colloidal QDs via shell growth, composition, and interfacial layers between the core and shell on the optoelectronic properties of QDs will be presented. Finally, the integration of optimized colloidal QDs into clean energy technologies such as photovoltaics, green hydrogen production systems and smart agriculture technologies will be presented, and possible pathways for future innovation and commercialization will be outlined.

T730412

PAIRING MICROBIAL ANALYSIS WITH CHEMICAL QUANTIFICATION: THE PERFECT WINE PAIRING? **Lauren L. Grant***; Clarissa S. Sit. Saint Mary's University, Department of Chemistry, 923 Robie Street, Halifax, NS B3H 3C3, Canada (clarissa.sit@smu.ca).

Terroir is a term used to describe the influences that a local environment has on the flavour of wine produced by individual vineyards. The impact that microorganisms in the soil, on the grapes and in the winery have on a wine is known as microbial terroir. For spontaneously fermented wines, which rely on naturally occurring microorganisms rather than the addition of yeast cultures, microbial terroir is of particular interest. Herein, we will present an analysis of the microbial terroir of L'Acadie

Vineyards, Nova Scotia's first certified organic vineyard, by investigating links between vineyard microbial populations and spontaneous Petillant Naturel (PetNat) wine fermentation. Microorganisms were isolated from vineyard grapes and winery tanks, cultured and purified in vitro and genotyped via Sanger sequencing. These findings were compared to shotgun metagenomic sequencing and taxonomic profiling of wine lees from two vintages. Chemical analysis of the PetNat was performed using HILIC-QTOF-MS to quantify key sugars and organic acids and assess variation between vintages, in order to determine whether those variations might correlate with changes in the microbial population. We propose that combining microbial fingerprinting with chemical analysis could help wineries identify fermentation-relevant and desired microbes, as well as spoilage risks.

T82015

PERTURBATIONS IN LIVER METABOLISM IN AN MPS II MOUSE MODEL REVEALED BY COMBINED PROTEOMICS AND METABOLOMICS. **Lekha Sleno***; Nathan Ghafari; Maggy Lépine. Department of Chemistry, UQAM, PO Box 8888, Downtown Station, Montreal, QC, H3C 3P8, Canada (sleno.lekha@uqam.ca).

Hunter syndrome, or MPS II, is a rare disease caused by a deficiency in iduronate sulfatase (IDS), resulting in the lysosomal accumulation of glycosaminoglycans (GAGs), dermatan and heparan sulfate. An approach combining proteomics and metabolomics by untargeted LC-MS/MS workflows was employed to highlight metabolic variations caused by MPS II in liver samples from an IDS knock-out mouse model. Some known perturbations showed similarities to previous reports in human patients, including altered levels of dimethylarginine, as well as disruptions in purine and amino acid metabolism. Correlation analyses combining the quantitative results from 3395 proteins and 383 metabolites allowed specific biological pathways to be highlighted in this complex dataset, including those involved in acyl-carnitine metabolism and oxidative stress. Additionally, 30 changing lysosomal proteins are implicated in lysosome organization and degradation. This work indicated that typical enzyme replacement treatment did not reverse most of the observed metabolic perturbations in this disease model.

T71001

(2026 GERHARD HERZBERG AWARD LECTURE) SEEING IS REALLY BELIEVING: THE REMARKABLE POWER OF NATIVE ELECTROSPRAY IONIZATION MASS SPECTROMETRY WHEN PROBING METALATION OF HUMAN METALLOTHIONEINS. **Martin J. Stillman***. Department of Chemistry, The University of Western Ontario, London, Ontario, Canada. (Martin.Stillman@uwo.ca).

Metallothioneins (MTs) are widely distributed in humans and are unusual in that despite the presence of 20 reduced cysteinyl thiol groups, they lack predefined metal ion binding sites. While the metallation properties of MTs with Zn(II) and Cd(II) are well known, involving the formation of

characteristic two-domain structures with exactly seven metal ions, the structures at other stoichiometries and with Cu(I), As(III) and Bi(III) are much less well defined. Equilibrium, and time-dependent and temperature-dependent kinetic studies using native ESI MS methods have revolutionized speciation analysis for the stepwise metallation pathways. Metallation reactions with Cu(I), As(III), and Bi(III) provide insight into the remarkable properties of MTs. Cu(I) forms a range of small clusters with the 20 cysteinyl thiolates, however, the exact sequence of the cluster formation between the two domains was only recently determined by using a combination of ESI-MS and excited state phosphorescence lifetimes. Reaction pathways of As(III) and Bi(III) with each of the three prominent human MT isoforms were studied using ESI-MS, X-ray absorption spectroscopy, and stopped flow kinetic methods. DFT calculations have supported structural assignments

T840616

ELECTROPOLYMERIZATION OF AU NANOPARTICLE INCORPORATED POLY(DOPAMINE) THIN-FILMS AT A MICRO LIQUID|LIQUID INTERFACE. **Jane Stockmann***. Department of Chemistry, Memorial University of Newfoundland, Core Science Facility, 45 Arctic Avenue, St. John's, NL A1C 5S7, Canada (tstockmann@mun.ca).

Dopamine (DA) is a critical biomolecule of the central nervous system (CNS) as well as a monomer incorporated into melanin, including eu-, pheo- and neuromelanin. Herein, we have investigated the electropolymerization of DA at a micro interface between two immiscible electrolyte solutions (micro-ITIES) between water|1,2-dichloroethane (w|DCE) to form polydopamine (PDA). Two electrodes, one immersed in either phase were used to control the wϕ. In this system, DA(aq) acts as an Galvani potential difference across the ITIES, ϕw – ϕo = ΔDCE electron donor while an ionic liquid composed of trihexyltetradecylphosphonium (P66614+) paired with $AuCl_4^-$ and dissolved in the DCE phase behaves as an electron acceptor. In this way, $AuCl_4^-$ is reduced forming Au nanoparticles. High pH was discovered to favour Au NP/PDA electrosynthesis creating a delicate, free-standing film. Au NP/PDA was used to modify a glassy carbon electrode (GCE) and employed as a DA (bio)sensor.1 This proof-of-concept DA-biosensor demonstrated quasi-reversible DA oxidation and a good limit-of-detection (LOD) and linear dynamic-range of 0.27 μM and 0.2-20 μM, respectively, using differential pulse voltammetry (DPV).

T91073

NMR INVESTIGATIONS OF MACROMOLECULAR POLYANION INHIBITORS. **R.M. Scott***[1]; Hemant K. Saini [2,3]; A. Louise Creagh [3]; Chanel C. La [2]; Irina Chafeeva [2]; David Thiam En Lim [1,2] Charles A. Haynes [3]; Simcha Srebnik [3]; Jayachandran N. Kizhakkedathu. [1] Department of Chemistry, University of British Columbia, 2036 Main Mall, Vancouver, BC, V6T 1Z1, Canada; [2] Center for Blood Research, Life Sciences Institute, University of British Columbia,2350 Health Sciences Mall, Vancouver, BC, V6T 1Z3, Canada; [3] Department of Chemical and Biological

Engineering, University of British Columbia, 2360 East Mall, Vancouver, BC, V6T 1Z3, Canada; [4] Department of Pathology and Laboratory Medicine, University of British Columbia,2350 Health Sciences Mall, Vancouver, BC, V6T 1Z3, Canada; [5] The School of Biomedical Engineering, University of British Columbia, 2350 Health Sciences Mall, Vancouver, BC, V6T 1Z3, Canada 6 Institut für Chemie und Biochemie, Freie Universität Berlin, 14195 Berlin, Germany (sstraus@chem.ubc.ca).

A number of biomacromolecules involved in the blood coagulation cascade are highly anionic. Heparin (UFH), a linear polysaccharide, is mostly known for its anticoagulant activity and is used in hospitals for the prevention and treatment of pulmonary embolism, deep venous thrombosis, coronary artery disease, heart valve diseases, and stroke1. Polyphosphates (polyP), released by activated platelets, promote coagulation and thrombosis2. Recent work has led to the development of Universal Heparin Reversal Agents or UHRAs3 or Macromolecular Polyanion Inhibitors (MPIs)4, to target UFH and polyP, respectively. This contribution examines how NMR (e.g. titrations, DOSY) was used to gain insight into molecular level interactions between UFH and UHRA-75, as well as between polyP and MPI-8. The implications of these findings in terms of the design of next generation macromolecular polyanion inhibitors will be presented.

P750645

PHOTOREACTIVE BIOCHAR NANOMATERIALS FOR ENHANCED ANALGETIC DECONTAMINATION PATHWAYS. **Zoe Sturmy***[1]; Judy MacInnis [2]; Stephanie MacQuarrie [2]; Geniece Hallett-Tapley [1]. [1] St. Francis Xavier University, Department of Chemistry, 5009 Chapel Square, Antigonish, NS B2G 2W5,Canada; [2] Cape Breton University, Department of Chemistry,1250 Grand Lake Road, Sydney, NS, B1M 1A2, Canada. (x2023aha@stfx.ca).

Analgesics are among the most widely consumed pharmaceuticals worldwide. However, their release into aquatic environments via hospital, domestic, and pharmaceutical effluents is poorly addressed by conventional wastewater treatment processes. As a result, novel remediation strategies are required. Photocatalytic approaches are promising due to their reliance on abundant, low-cost energy sources and the potential for catalyst reuse. Photodegradation has proven effective for the remediation of various pharmaceutical contaminants, including hormones, antibiotics, antidepressants, and, in this work, analgesics. Previous studies at StFX have demonstrated that light-activated nanomaterials can successfully remediate a broad range of antibiotics. Building on this foundation, the current contribution will discuss recent advances of environmentally conscious photocatalysts based on gold nanoparticle-functionalized crab biochar for the photodegradation of common analgesics. Target compounds include over-the-counter NSAIDs such as ibuprofen (Advil™) and diclofenac (Voltaren™), as well as prescription painkillers ketorolac (Toradol™) and tramadol, which are frequently detected downstream of medical, municipal, and manufacturing sources. Crab biochar synthesis, in collaboration with the MacQuarrie Group at Cape Breton University, affords a value-added material stream – converting discarded waste products that comprise ~30% of the snow crab industry. Gold nanoparticles are synthesized via an eco-friendly, starch-based method.

Combined adsorption and visible-light activation afford an opportunity for effective, on-site water treatment while avoiding ecosystem disruption of high-energy UV irradiation.

T930511

SURFACE FORCES AND NANOSCALE CHEMISTRY IN PLANT MICROBE INTERACTIONS. **Ruby Sullan***. University of Toronto Scarborough, Department of Physical and Environmental Sciences, Department of Chemistry, 1065 Military Trail, Toronto, ON M1C 1A4, Canada (ruby.sullan@utoronto.ca).

The nano-bio interface plays a central role in shaping how microorganisms interact with both living and non-living surfaces, with important implications for beneficial and detrimental processes in agricultural systems. In this talk, I will present two complementary studies that use analytical methods to probe these interfacial interactions at the nanoscale. In the first, atomic force microscopy-based single-cell force spectroscopy, supported by fluorescence imaging, was used to quantify the early attachment of plant growth-promoting rhizobacteria to different regions of Arabidopsis thaliana roots. These measurements revealed strain-dependent adhesion strategies involving micrometer-scale surface polymers, distinct roles of flagella, and contributions from electrostatic, hydrophilic, and hydrophobic interactions.[1] In the second study, I will show how positively charged amine-modified polystyrene nanoplastics disrupt this beneficial interface by forming stable coatings on bacterial cells, reducing viability, and impairing root colonization, with the extent of these effects strongly influenced by the growth environment.[2] Together, these results demonstrate how analytical measurements at interfaces can reveal both the mechanisms that support beneficial root colonization and the pathways through which emerging contaminants disrupt these interactions.

T741019

FROM DELIVERY TO MEASUREMENT: INVESTIGATING THE INTRACELLULAR FATE OF QUANTUM DOT-BASED CONCENTRIC FRET PROBES FOR CELLULAR ANALYSIS. **Agnes Szwarczewski***; Jasmine Bernal Escalante; W. Russ Algar. University of British Columbia, Department of Chemistry, Vancouver, BC V6T 1Z1, Canada. (aszwarcz@chem.ubc.ca).

Förster resonance energy transfer (FRET)-based probes are promising tools for bioanalysis. Concentric FRET (cFRET) is a design strategy enabling multiplex detection of biological targets using a single probe, wherein multiple copies of multiple dye acceptors are assembled onto a central quantum dot (QD) donor through biomolecular linkers (e.g., peptides) [1]. Compared to conventional QD-based FRET probes, a single cFRET probe avoids potential challenges with differential intracellular delivery, distribution, or stability, making it well-suited for studying intracellular pathways. However, cFRET systems have thus far been limited to “test tube” formats [1], and their

translation into the intracellular environment remains a key challenge. Here, we report efforts in advancing cFRET probes toward intracellular analysis. We developed a new cFRET configuration combining yellow-emitting QDs with red- and deep-red-emitting dye acceptors. Following cytosolic delivery via microinjection into live cells, probe distribution and photoluminescent stability were evaluated using fluorescence microscopy. Temporal decreases in FRET signals were observed, prompting a systematic investigation of contributing factors, including non-specific intracellular probe degradation and bioconjugation strategies. This study provide an essential foundation towards rational design of QD-based multiplex sensors for cellular analysis.

T830313

SULFUR ISOTOPES FROM MEASUREMENT TO INTERPRETATION IN ARCHAEOLOGY. **Damon Tarrant***. Michael Richards. Department of Archaeology, Simon Fraser University, 8888 University Drive, Burnaby British Columbia V5A1S6 (Dtarrant@sfu.ca).

Isotope ratios of human and animal tissues (mainly teeth and bones) are routinely used in archaeology, ecology, and forensic sciences to study past diets, mobility, and climate. These studies have mainly used carbon, nitrogen, strontium and oxygen; however researchers are also increasingly measuring sulfur isotope ratios to study past diet and mobility. Sulfur is relatively difficult to measure in mammal tissues, specifically bone collagen (the main substrate used for most of these studies) as it is present in very low (0.16%) amounts. Recent analytical developments have now enabled the simultaneous measurement of carbon, nitrogen, and sulfur isotopes in small (1.5mg) mammal bone collagen. In our talk we will present the results of our applications of sulfur isotope measurements for studying mobility and migration studies in a range of archaeological contexts. We have also constructed sulfur isotope abundance maps (isoscapes) from different global locations to explore how different environmental processes influence the spatial distribution of sulfur isotopes and how these processes may change over time due to anthropogenic impacts. Finally, we examine how statistical models can be used for high-resolution mobility studies and how sulfur may complement the more established strontium- and oxygen-based mobility studies.

T830611

INKJET-PRINTED SERS SENSORS FOR FIELD CHEMICAL ANALYSIS. **Li-Lin Tay***; Hal Bowen-Smith; Ali Ghaemi; Greg Wardle; John Hulse. National Research Council Canada, Metrology Research Centre, Ottawa, ON Canada K1A0R6 (lilin.tay@nrc-cnrc.gc.ca).

Development of a robust, rapid and sensitive technology for the detection and identification of chemicals and biological agents such as contraband substances, narcotics and toxins will provide a critical decision making advantage for first responders and military personnel. Recent advances in nanofabrication, microelectronics and computational power have enabled miniaturization of many

instruments. Among the many portable analytical instruments, handheld Raman spectrometers has become quite common. . Coupled with Surface Enhanced Raman spectroscopy (SERS), which is known for its enormous sensitivity, Raman analysis is well suited for many field detection challenges. In this presentation, we will demonstrate the fabrication and analysis of paper-based SERS sensors through inkjet printing of colloidal Au nanoparticles (AuNP) onto paper substrate. These flexible and porous paper-based SERS sensors not only fulfill the cost effectiveness and robustness criteria, they have the additional advantage of the point-of-sampling capability that is lacking in the rigid SERS sensors. With their inherent filtration sampling capability, we show the use of paper SERS sensors for the detection of chemical aerosols. We will also present the use of a precision materials printer to deposit quantifiable amounts of fentanyl uniformly across the active sensing area of a paper SERS sensor. This will allow for analyte loaded references to be prepared and used in the field as standards for comparison.

T840118

DEVELOPMENT AND APPLICATION OF A PFAS (PER- AND POLYFLUOROALKYL SUBSTANCES) DECONTAMINATION PROTOCOL FOR ULTRA-TRACE ANALYSIS. **Manda Tchonlla***; Jessica L. Bennett; Graham A. Gagnon. Centre for Water Resources Studies, Department of Civil & Resource Engineering, Dalhousie University (tmanda@dal.ca).

Ambient organofluorine contamination from laboratory consumables, reagents and analytical instrumentation routinely creates interference and jeopardizes data quality in ultra-trace level PFAS analysis. Here, we present a comprehensive decontamination protocol designed to mitigate PFAS contamination throughout sample processing and LC-MS/MS analysis and demonstrate its application through a modified EPA Method 533 workflow. Initial evaluation of reagents and consumables showed that methanol (used in sample processing and LC-MS/MS analysis) was the most common contributor of PFAS contamination, with 6:2 FTS and PFBS being the most often detected compounds. Validation studies confirmed effective removal of PFAS contamination from laboratory materials and reagents, and when applied to the full analytical workflow, the protocol enabled reliable quantitation of 23 PFAS with method detection limits of 0.1-0.4 ng/L. The method was then applied in a field sampling program, where QA/QC protocols confirmed that contamination control remained effective under real-world sampling conditions. This work delivers a practical, reproducible framework for ultra-trace PFAS analysis that directly supports the reliability demands of environmental monitoring programs and regulatory compliance

T830111

A NOVEL METHOD TO EXTERNALLY ADJUST COLUMN LENGTH DURING GAS CHROMATOGRAPHY OPERATION. **Kevin B***; Thurbide; Kade L. Shepherd. Department of Chemistry, University of Calgary, 2500 University Dr. NW, Calgary, AB, T2N 1N4, Canada (thurbide@ucalgary.ca).

A method for externally adjusting the column length during gas chromatography (GC) operation is introduced. The technique employs the controlled dehydration of a water stationary phase off a stainless-steel capillary column wall, which is then removed by the carrier gas. By strategically halting the dehydration/rehydration process, partially coated column lengths are created as desired. Good stability is achieved in maintaining new column lengths for most settings examined. Analyte retention reproducibility, the dynamics of the process, and application of the technique will be presented and discussed.

T930615

STRAIN-INDUCED ULTRASTRUCTURAL REMODELING OF COLLAGEN: A POLARIZATION-RESOLVED SECOND HARMONIC GENERATION MICROSCOPY STUDY. **Danielle Tokarz***[1]; MacAulay Harvey. Department of Chemistry, Saint Mary's University, 923 Robie Street, Halifax, NS, B3H 3C3, Canada 2Department of Physics and Atmospheric Science and School of Biomedical Engineering, Dalhousie University, Halifax, NS, B3H 4J5, Canada (danielle.tokarz@smu.ca).

Advancements in analytical science and molecular spectroscopy are essential for interpreting the relationship between tissue structure and function. Nonlinear optical microscopy, in particular, second harmonic generation (SHG) microscopy, can provide intrinsic tissue ultrastructural information in a completely non-invasive way. For instance, SHG microscopy has been used to visualize and structurally interrogate several types of fibrillar arrangements present in biological animal tissue, revealing nanoscale structural parameters in collagen.

To obtain structural information about the assembly of fibrillar structures, modulation of the linear polarization of the incoming laser light and discrimination of the polarization of the outgoing SHG signal is performed using a technique referred to as polarization-in, polarization-out (PIPO) SHG microscopy. This measurement allows the extraction of several parameters that can be directly related to the organization of the fibrillar structures. In the present study, we use PIPO SHG microscopy to investigate the ultrastructural changes that occur to individual collagen fibrils when they are stretched. A change in the ultrastructural parameter related to the helical pitch angle was found. This likely results from the unwinding of the collagen triple helix with strain demonstrating that SHG microscopy is sensitive to molecular reconfiguration.

T730513

RECENT DEVELOPMENTS IN TOOLS FOR HIGH-TEMPERATURE AQUEOUS ELECTROCHEMISTRY. **Muna Abdulaziz***[1]; Kostyantyn Pichugin [2]; Travis Whistle [1]; Tetyana Maksyuta [2]; German Sciaini [2]; Liliana Trevani [1]. [1] Faculty of Science, Ontario Tech University, 2000 Simcoe St North, Oshawa, Ontario, L1G 0C5, Canada; [2] Department of Chemistry, University of Waterloo, 200 University Ave West, Waterloo, Ontario,N2L 3G1, Canada (liliana.trevani@ontariotechu.ca).

Advances in high-temperature and high-pressure (high-T,p) experimental techniques in solution chemistry have enabled the study of complex chemical processes under extreme conditions.1,2 Yet, progress in electrochemical methods remains primarily confined to autoclave and corrosion studies, as well as pH and potential measurements,2,4, with a few studies involving hydrodynamic electrodes.5,6 Here, we address this gap by integrating a small-channel flow cell with specially designed thin-film electrodes for high-T,p applications.7 This new system provides precise control of mass transfer and enhanced current responses at temperatures up to 160 °C and pressures up to 65 bar.7 The cell design is also compatible with electrochemical Raman, enabling, in the future, simultaneous analysis of reaction mechanisms and electrode surface processes under extreme conditions.

P750731

DEVELOPING AND CHARACTERIZING CONTACT-DRAWN COMPOSITE SPIDER SILK-COLLAGEN FIBRES. **Yanitza Trosel***. Department of Chemistry, Dalhousie University, Chemistry Building, 6274 Coburg Road, Halifax, NS B3H 4R2, Canada (yanitza.trosel@dal.ca).

Spider silk fibres are desirable due to their remarkable mechanical properties, including high strength, extensibility, and durability in different environmental conditions. Spider silk fibres are composed of proteins called spidroins, with structural features that combine to provide outstanding mechanical performance. Their high strength, extensibility, biodegradability and biocompatibility make them promising candidates for biomaterial applications. Recombinant production of spidroins provides a scalable and tunable alternative to natural silk harvesting, enabling controlled modification of protein sequence and material properties. In this work, we investigate the structure–property relationships of composite spidroin and collagen-based fibres produced via contact drawing. In contact drawing, fibres are drawn from a viscous solution using a pin, creating a liquid bridge that stretches into a fibre, promoting molecular alignment. A combination of wide-angle X-ray diffraction (WAXD), Fourier-transform infrared spectroscopy (FTIR), tensile testing, and magic-angle spinning (MAS) solid-state NMR are used here to probe molecular structure, secondary structure content, and mechanical performance.

T82097

EXPLORING ‘FOREVER CHEMICAL’ CONTAMINATION IN PRINCE EDWRAD ISLAND DRINKING WATER SOURCES. **Nicole Unterlander***; Kelsey Jordan; Adriana Catalli; Bouchaib El Bahh; Anja Vogt. National Research Council Canada, Aquatic and Crop Resource Development, 550 University Avenue, Charlottetown, PE, C1A 4P3, Canada (nicole.e.unterlander@gmail.com).

Per- and polyfluorylalkyl substances (PFAS) are a class of synthetic organic compounds with exceptional chemical stability and resistance to heat, oil/grease, and water. PFAS are used in

production of various products including textiles, paint, sealants, medical devices, food packaging, cosmetics, fire extinguishing foam, and electronics [1]. Their strong C-F bonds, surfactant properties, and high water solubility mean they are persistent and mobile contaminants, accumulating in water, food, and landfills [2]. PFAS have been the subject of increasing scientific and political scrutiny due to links to negative health outcomes including cancer, endocrine disruption, and immunological, neurological, and reproductive issues [2]. Quantitation poses unique analytical challenges like 1) high background contamination due to environmental ubiquity, 2) vast chemical diversity (>10,000 PFAS), 3) strong adsorption onto glass and metals, and 4) ultra-trace (≤ppt) concentrations in samples. We have developed a clean, reproducible method for the quantitation of 33 select PFAS (the most common and toxicologically relevant [3]) in ocean and drinking water samples (500 ml). A study to demonstrate method effectiveness was performed on samples from 3 municipally-treated drinking water sources in PEI (Charlottetown, Cornwall, Stratford) and 1 'rural' well-water source (Brackley). The method LODs range from 0.05 – 10 ppt, with recoveries ≥74.6%.

T91033

INVESTIGATION OF ELEMENTAL DISTRIBUTION IN BONE USING LA-ICP-MS AND X–RAY SPECTROSCOPY. **Cassidy VanderSchee***. The King's University, Department of Chemistry, 9125 50 St NW, Edmonton, AB T6B 2H3, Canada. (cassidy.vanderschee@kingsu.ca).

Bone tissue is a well-known sink for various essential and toxic trace metals. Local distribution of these elements within bone tissue can provide detailed information on local exposures, uptake mechanism, and exposure timeline; information which traditional bulk quantification methods fail to capture. Synchrotron radiation micro X-ray fluorescence (SR-μXRF) and laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) were used as complementary methods to determine the elemental bone distribution in two scenarios: A) tungsten (W) in mouse femoral bone after oral exposure to aqueous tungsten, and B) lead (Pb) in archeological 18th/19th century bone tissue from the British Royal Navel cemetery in Antigua. While XRF provides non-destructive, quick imaging and the ability to be paired with X-ray Absorption Spectroscopy for speciation determination, resolution and quantification is limited by the heterogeneity of the bone tissue. LA-ICP-MS, a destructive surface technique, improves sensitivity while allowing for quantification and high-resolution images. Used together, these techniques reveal that localized concentrations of tungsten and lead are enriched in bone at concentrations substantially higher than indicated by bulk measurements, with implications for uptake mechanism, toxicity, and lifetime exposure of these elements.

T81011

COMPARISON OF MICROSAMPLING AND MICROEXTRACTION FOR OXYLIPIN ANALYSIS. **Dajana Vuckovic***; Arianna Cirillo. Department of Chemistry and Biochemistry, Concordia University, 7141 Sherbrooke Street West, Montréal, QC, Canada H4B 1R6. (dajana.vuckovic@concordia.ca).

Microsampling approaches, including volumetric absorptive microsampling (VAMS) and volumetric dried blood spot (DBS) collection, have emerged as effective strategies for minimally invasive, low-volume sampling for lipidomics. These techniques reduce participant burden, enable high-frequency longitudinal sampling, and support decentralized and at-home study designs. Concurrent advances in microextraction methodologies, particularly solid-phase microextraction (SPME), have further enhanced lipidomics workflows by simplifying sample preparation and improving matrix clean-up and limits of detection from limited sample volumes. In this study, we systematically compared DBS, volumetric DBS, VAMS, and SPME for targeted oxylipin profiling in terms of recovery, repeatability and matrix effects. The effects of extraction device selection and post-collection storage conditions on analyte stability were also examined. Finally, these emerging workflows were compared with conventional plasma collection followed by C18 solid-phase extraction for oxylipin analysis, providing practical guidance for selecting the most appropriate sampling and extraction strategy for specific applications.

T730111

GLUTARALDEHYDE-CROSSLINKED ENZYMES FOR DIGESTION OF DRIED PROTEINS. **Karen Waldron***; Marie-Pier Ouellet. Université de Montréal, Campus MIL, 1375 av. Thérèse-Lavoie-Roux, Montréal QC H2V 0B3, Canada (karen.waldron@umontreal.ca).

Proteolytic enzymes immobilized by glutaraldehyde (GA) crosslinking enable rapid protein digestion during sample preparation while resisting autolysis. We previously optimized GA-crosslinked trypsin and chymotrypsin for in-solution digestion under ideal aqueous conditions with activities comparable to soluble enzymes. However, these conditions do not reflect applications requiring digestion of dried proteins on surfaces (tissue sections, glass slides, or dried blood spots). This work aims to adapt GA-immobilized trypsin for quasi solid-phase digestion. GA-crosslinked trypsin particles are prepared by controlled addition of 2.5% GA to trypsin in phosphate buffer, followed by washing and glycine capping. Because the resulting particles are soft and polydisperse, we first optimized deposited particle mass and drying time using a UV assay with the synthetic substrate BAEE. Enzymatic activity was then evaluated for digestion of β-casein (native) and lysozyme (denatured and alkylated). Substrates were deposited on glass slides and MALDI plates and digested for 4 hours, with parallel batch digestions as controls. Digestion efficiency was assessed by comparing peptide maps by CE-UV and MALDI-MS after solubilizing spots. The effects of substrate concentration, deposited volume, wetting conditions, digestion time, and enzyme mass were examined. Achieving equivalent enzyme-to-substrate ratios between quasi solid-phase and batch digestions remains challenging. Implementation of a peptide internal standard is underway to

normalize peptide responses and improve quantitative assessment of enzymatic activity under quasi solid-phase conditions.

T741018

A MAGNETIC NANOPARTICLE BASED METAL ENHANCED FLUORESCENCE PLATFORM FOR QUANTIFYING EXTRACELLULAR VESICLES. **Isabella Walker***; Huiyan Li. College of Engineering, University of Guelph, 50 Stone Rd E, Guelph, ON N1G 2W1, Canada. (walkeri@uoguelph.ca).

Cancer is the second leading cause of death worldwide, and early detection is critical for improving patient outcomes. Extracellular vesicles (EVs) are promising non-invasive biomarkers secreted from cancer cells into biofluids such as blood; however, current detection methods lack sufficient sensitivity for low-abundance cancer EVs present at early stages of the disease. Although metal-enhanced fluorescence (MEF) improves signal intensity, limited reaction surface area and inefficient mass transfer restrict EV capture and overall assay performance. To overcome these challenges, this research developed a magnetic-nanoparticle-based MEF platform to quantify EVs in blood plasma, achieving high sensitivity through integrating MEF with increased reaction surface area and improved mass transfer. EVs isolated by size exclusion chromatography from the human ovarian cancer cell line OVCAR-3 were tested. Surface chemistry of the nanoparticles and immunoaffinity capture conditions were optimized to maximize reproducibility and efficiency. The results showed that the nanoparticles with MEF provided a 5.3-fold higher signal than non-MEF nanoparticles, with the assay limit of detection at least one order of magnitude higher than conventional methods, indicating enhanced EV detection. This platform significantly improves EV capture and fluorescence signal, offering a sensitive approach for early cancer biomarker detection from small-volume blood samples.

T830714

CONFORMATION DYNAMICS AS AN EXPLANATION FOR THE PROSMICUITY OF AMI-DOMAIN IN INTEGRIN MAC-1. **Heather Couture***; Xu Wang. School of Molecular Sciences, Arizona State University, Tempe, Arizona, USA (xuwang@asu.edu).

Sciences, Arizona State University, Tempe, Arizona, USA.

β2 integrins are integrin adhesion receptors expressed exclusively on leukocytes. Despite strong structural homology and identical ligand binding mechanisms in their ligand binding α I-domains, the ligand specificities of these integrins are very different. In particular, αLI-domain binds only for a handful of proteins while αMI-domain are highly promiscuous. We showed that the promiscuity of αMI-domain is the result of its high affinity for carboxyl groups, a consequence of its low affinity for the ligand-chelating Mg2+ ion. To understand the reason for the differences in the Mg2+ affinities of α I-domains, we investigated the dynamics of αMI-domain and αLI-domain. Our data show that,

although the two domains have similar picosecond and nanosecond dynamics, αMI-domain has considerably more millisecond dynamics around its metal-binding site. In addition, Mg2+ produced significant increases in the dynamics of αMI-domain's α7 helix, and the addition of glutamate, a known ligand of αMI-domain, increased the dynamics further. We think that the intrinsic dynamics in αMI-domain allowed it to bind carboxyl groups with higher affinity, and ligand-binding induced additional dynamics that led to easier activation of the domain, resulting in its promiscuity.

T92057

ECL-BASED ABSOLUTE QUANTUM EFFICIENCY & MOLECULAR KINETICS STUDY OF A NEW CLASS OF BORON- AND NITROGEN-EMBEDDED POLYCYCLIC AROMATIC HYDROCARBONS (PAHS). **Tianyu Wei***[1]; Deng-Tao Yang [2]; Zhifeng Ding [1]. [1] Department of Chemistry, Western University, 1151 Richmond St, London, ON N6A 3K7, Canada; [2] School of Chemistry and Chemical Engineering, Northwestern Polytechnical University, Xi'an, Shaanxi 710072, China (twei56@uwo.ca).

For the first time, this work reports the determination of absolute electrochemiluminescence (ECL) quantum efficiency (ΦECL) and molecular kinetics for a new class of boron (B)- and nitrogen (N)-embedded polycyclic aromatic hydrocarbons (PAHs), represented by structural analogues BN2 and BN1.[1] Absolute ΦECL was quantified from the ratio of total emitted photons to total electrons consumed, using a laboratory-designed instrument capable of directly measuring photon and electron fluxes with a MATLAB-based program. BN2 achieved a maximum absolute ΦECL of 0.070 ± 0.001% via the coreactant pathway with tri-n propylamine (TPrA), exhibiting an efficiency approximately 700 times greater than BN1 despite differing by only one boron atom. This striking contrast highlights the decisive role of B–N bonding in modulating the HOMO–LUMO gap and ECL efficiency.[1] For the molecular kinetics study, time-resolved ECL transients with nanosecond resolution were recorded using a laboratory designed instrument setup and analyzed by comparison with simulated transients with defined rate constants, generated using COMSOL finite-element modeling. The annihilation rate constants for both analogues were determined to be $(1.2 \pm 0.1) \times 10^9$ $M^{-1} s^{-1}$, indicating very similar molecular kinetics. These results clearly decouple energy-level tuning from kinetic control, providing new mechanistic insight for the rational design of high-performance ECL luminophores.

T91034

210PB IN HUMAN TOENAILS: A BIOMARKER OF CUMULATIVE RADON EXPOSURE. **Michael Wieser***[1]; Kerri Miller [2]; Dustin Pearson [2]; Aaron Goodarzi [2]. [1] Department of Physics and Astronomy, University of Calgary. 2500 University Dr. NW, Calgary, AB T2N 1N4, Canada; [2] Department of Biochemistry and Molecular Biology, Cumming School of Medicine, Arnie Charbonneau Cancer Institute, University of Calgary. 3280 Hospital Dr. NW, Calgary, AB, T2N 4Z6, Canada (mwieser@ucalgary.ca).

Long-term exposure to indoor radon is a major public health concern, yet there is currently no reliable biomarker of cumulative exposure. Here we investigate whether 210Pb incorporated into human toenails can serve as a record of long-term radon exposure in the built environment. Toenail clippings from 67 individuals with well-characterized residential radon histories and environmental time-activity patterns were analyzed for 210Pb by isotope dilution mass spectrometry using a multiple-collector inductively coupled plasma mass spectrometer. Participants residing in high-radon environments exhibited a mean 210Pb-to-total Pb ratio of 0.298 fg/ng, compared with 0.075 fg/ng among those in low-radon environments. These results suggest that 210Pb incorporated into toenails may provide a measurable record of cumulative radon exposure. More broadly, the study highlights the potential of isotopic measurements in keratinous tissues as forensic indicators of environmental exposure, complementing traditional elemental analyses and offering new opportunities to reconstruct long-term exposure histories.

T91083

(VIRTUAL) DEVELOPMENT AND VALIDATION OF A METHOD FOR VITAMIN B12 DETERMINATION IN DIETARY SUPPLEMENTS AND NUTRITIONAL YEAST BY HPLC-ICP-MS. **Mesay M. Wolle***. Office of Chemistry and Toxicology, Office of Analytical Operations and Applied Science, Human Foods Program, U.S. Food and Drug Administration, 5001 Campus Drive, College Park, MD 20740, USA (Mesay.Wolle@fda.hhs.gov).

Vitamin B_{12} is comprised of multiple cobalt-containing tetrapyrrole complexes including cyano-, hydroxy-, methyl-, and adenosyl-cobalamin. It plays a key role in red blood cell formation and functioning of the brain and nervous system. Naturally occurring cobalamins are only found in animal-derived foods, including meat, eggs and dairy. Fortified foods and dietary supplements can be used to increase vitamin B12 intake. Accurate quantification of all forms of vitamin B_{12} is essential for verifying label claims and ensuring regulatory compliance. Traditional analytical techniques such as microbiological assays, radioisotopic methods, and spectrophotometry lack sufficient sensitivity and/or specificity to the different B12 complexes. This presentation will cover the development and single laboratory validation of an HPLC-ICP-MS method for determining vitamin B12 in dietary supplements and nutritional yeast. The HPLC-ICP-MS technique offers specific and independent measurement of each cobalamin structure, with robust elemental selectivity by quantifying the central cobalt atom. Method performance was evaluated for accuracy and precision in dietary supplements (tablet, capsule, chewable, lozenge, nugget, gummy, powder and liquid) and nutritional yeast samples fortified at 50%, 100% and 200% of their native analyte (cyano-, hydroxy-, methyl-, or adenosyl-cobalamin) mass fraction in duplicate, which was conducted in accordance with FDA's Guidelines for the Validation of Chemical Methods.

T92096

CHOOSING THE RIGHT NEBULIZER FOR YOUR ICP-OES APPLICATION. **Alejandro Amorin***; Longbo Yang. Agilent Technologies, #5, 6705 Millcreek Drive, Mississauga, ON L5N 8B3, Canada (longbo.yang@agilent.com).

Selecting the ideal nebulizer is a critical step in optimizing Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES) performance, as it directly influences sensitivity, stability, and long-term reliability. With a wide array of designs available, matching the hardware to the sample matrix is essential for analytical success. This presentation provides a comprehensive guide to navigating the selection process by evaluating key performance factors such as sample matrix compatibility, aerosol efficiency, and operational robustness. By examining comparative data and real-world application examples, attendees will gain practical insights into which nebulizer configurations best suit their workflows. This session aims to empower analysts with the technical knowledge required to make informed, application-specific hardware choices that enhance overall data quality and laboratory productivity.

T92077

EXPERIMENTS IN CROWDED MACROMOLECULAR SOLUTIONS. **Anand Yethiraj***. Department of Chemistry, University of Guelph, 50 Stone Road East, Guelph, ON N1G 2W1, Canada (ayethira@uoguelph.ca).

Living cells are very crowded environments with large/small, charged/uncharged, hydrophobic/hydrophilic macromolecules. Knowing how individual proteins will behave in the presence of this crowding is challenging; indeed, even the nature of the crowding environment is often insu=iciently characterized. We use a bottom-up colloidal model approach -- and multiple experimental tools including NMR, rheology and neutron scattering -- to examine simple polymeric and colloidal crowders as well as more complex crowding environments such as lysed cells. We also examine the role of crowder charge and hydrophobicity. We use these di=erent experimental modalities to obtain quantitative information about crowding environments. Across di=erent systems, we find a surprising universality in the concentration dependence of macromolecular di=usivity, but we find that even simple questions, such as "what is the crowder packing fraction?" do not have unambiguous answers. A macromolecular crowding “status report” will be provided.

T81092

NON-TARGET LC–HRMS/MS METHODS FOR ANALYSIS OF CYANOBACTERIAL SECONDARY METABOLITES. **Lydia Zamlynny***[1,2]; Elliott J. Wright [2]; Rob C. Jamieson [1]; Daniel G. Beach [1,2]. [1] Centre for Water Research Studies, Dalhousie University, Halifax, NS, Canada; [2] Metrology Research Centre, National Research Council of Canada, Halifax, NS, Canada (lzamlynny@dal.ca).

Cyanobacteria are of global concern due to impacts on ecosystems and public health risk from production of bioactive secondary metabolites, including cyanotoxins, which exhibit acute mammalian toxicity. Comprehensive study of cyanobacterial metabolites is challenging due to the large number of compounds potentially being produced, leading to non-target analysis (NTA) methods being increasingly implemented. However, the quality of obtained results is often unclear due to a lack of reference materials and method evaluation raising concerns over the quality of generated results. Here, we present the development and evaluation of a NTA workflow for profiling of cyanobacterial metabolites using data-dependent LC–HRMS/MS acquisition and semi-automated processing to identify compounds of interest by product-ion, mass list, and spectral library searching. Performance was evaluated based on detection of cyanotoxins in a cyanobacterial matrix reference material. Further profiling of this material led to the identification of other peptide classes, expanding its class coverage and utility as a positive control. Lastly, the analysis of cyanobacterial samples led to detection of over 100 metabolites including previously undetected toxin analogues. The wider application of the established workflow will lead to a better understanding of the complex metabolite profiles produced by cyanobacteria as well as their associated risks.

T730515

SURFACE-CONFINED METAL-ORGANIC ELECTROCHROMIC MATERIALS. **Marjan Saedi***; Salma Jadali; E. Bradley Easton, Olena V. Zenkina. Ontario Tech. University (Olena.zenkina@ontariotechu.ca).

Electrochromic (EC) materials have attracted considerable attention for applications in displays, signage, wearable electronics, and adaptive camouflage. Despite substantial progress, conventional EC systems continue to suffer from limited durability, stability, and overall performance, underscoring the need for new design strategies and more robust material platforms. In this context, EC devices based on transition metal complexes that avoid the use of noble metals are particularly attractive, as they offer cost-effective solutions with colour tunability enabled through rational molecular design. Our group has developed a new class of efficient and robust metal–organic EC materials fabricated on surface-enhanced, conductive, screen-printed metal oxide supports. We demonstrated that tuning molecular structures (metal complexes or anchoring linkers) can define the colours and stability of electrochromic monolayers. Notably, the chemical nature of the linker plays a decisive role in dictating interfacial organization and long-term device stability. In this work, we introduce an on-surface click-chemistry strategy for constructing ultra-durable EC materials, which yields significantly enhanced robustness compared to our previously reported N-quaternization approach on siloxane templates. We further explore diazonium coupling and electrochemical deposition as alternative surface-functionalization routes, providing versatile pathways toward highly stable, surface-confined metal–organic EC systems with improved performance.

T740118

AMPLIFIED FLUORESCENCE DETECTION OF PROTEINS IN LIVE CELLS USING TARGET-INITIATED DNAZYME MOTORS. **Huyan Xiao***; Jeffrey Tao; Hanyong Peng; X. Chris Le; Hongquan Zhang. Division of Analytical & Environmental Toxicology, Department of Laboratory Medicine & Pathology, University of Alberta, Edmonton, Alberta, T6G 2G3, Canada. (hongquan@ualberta.ca).

Inspired by endogenous protein motors, researchers have developed various synthetic DNA motors that mimic the walking behavior of protein motors along a track. However, the application of DNA motors for in situ signal amplification in live cells remains limited due to low mobility, challenges in real-time monitoring, and inefficient cellular uptake. Here, we report target-initiated DNAzyme motors for amplified detection of specific proteins in live cells. To enhance signal amplification, nanoparticles were used as scaffolds to assemble hundreds of DNA track strands on a single particle, enabling the activation of hundreds of fluorophore molecules in response to a single target-binding event. Target recognition domains were incorporated into the motor design to achieve protein-specific activation. Autonomous motor operation was enabled by DNAzymes, allowing self-powered walking without the need for protein enzymes. We demonstrate this strategy for the amplified detection of apurinic/apyrimidinic endodeoxyribonuclease 1 (APE1), a base excision repair enzyme in HeLa cells, and human epidermal growth factor receptor 2 (HER2), a cancer biomarker expressed on the surface of breast cancer cells. These target-initiated DNAzyme motors expand the applications of DNA motors in molecular sensing, live-cell imaging, and molecular interaction analysis.

T930611

MODULATION OF PLASMONIC COUPLING AND SIGNAL PROPAGATION IN SURFACE-ENHANCED RAMAN SPECTROSCOPY BY DISSOLVED OXYGEN AND ORGANIC SOLVENTS. **Xu Zhang***; Collins Nganou. Department of Chemistry, Cape Breton University, Sydney, Nova Scotia, B1P 6L2, Canada (xu_zhang@cbu.ca).

Surface-enhanced Raman spectroscopy (SERS) enables ultrasensitive analyte detection through electromagnetic and chemical enhancement mechanisms that arise from plasmonic interactions at nanostructured surfaces. Here we demonstrate that dissolved oxygen acts as a strong attenuator of SERS signals in aqueous media. Chemical deoxygenation lowers the detection limit by 9–10 orders of magnitude, enabling single-molecule detection in approximately 300 µL of solution. Notably, oxygen removal also permits remote detection of analytes beyond the direct laser excitation region, with signal transmission observed over distances up to 1 m. We attribute this phenomenon to long-range plasmonic coupling within and between nanoparticle aggregates, facilitating propagation of enhanced electromagnetic fields throughout the sample volume. In addition, we investigate how organic solvents with varying dielectric constants influence SERS signal transmission. These findings

provide new mechanistic insights into environmental modulation of plasmonic coupling and its impact on analytical sensitivity.

T92097

LEVERAGING HIGH-THROUGHPUT ANALYSIS TO CHARACTERIZE THE FATE, OCCURRENCE, AND ATTENUATION OF 6PPDQ IN URBAN WATERS AT SCALE. Angelina Jaeger [1,2], Joseph Monaghan [1], Niki Gholamiaval [1,2], Haley Tomlin [3], Jamieson Atkinson [3], Chris G Gill [1,2], **Erik T Kroch*** [1,2]. [1] Centre for Health and Environmental Mass Spectrometry, Department of Chemistry, Vancouver Island University, Nanaimo, B.C., Canada; [2] Department of Chemistry, University of Victoria, Victoria, B.C., Canada; [3] British Columbia Conservation Foundation, Nanaimo, B.C., Canada (erik.krogh@viu.ca).

Para-phenylene diamine quinones (PPDQs) are an emerging class of acutely toxic contaminants derived from tire road wear particles associated with mass die-off events of salmonids in the Pacific Northwest. Characterizing the fate and distribution of PPDQs over complex urban landscapes requires widescale intensive sampling enabled by high throughput analytical workflows. Our group has pioneered a direct mass spectrometry approach using an on-line sample clean up via a capillary hollow fibre membrane immersion probe. We report on the method optimization providing a '*fit-for-purpose*' method for direct analysis 6PPDQ in complex waters. Key performance metrics include detection limits of ~ 1 ng/L with a complete analytical duty cycle of 3 mins/sample. Combined with a purpose-built smartphone sample collection app, low-cost auto-sampler, and data processing tools, we describe end-to-end automation that provides up to 200 samples/day and enables rapid reporting and adaptive sampling. We will present results from a large citizen science sampling campaign including over 7500 samples on Vancouver Island (BC, Canada) representing the single largest PPDQ dataset globally. Working with community and First Nation partners, we characterize spatiotemporal trends and environmental exposures in urban streams. This work has resulted in the identification of priority inputs and informed local mitigation efforts.

T91099

OPTIMISING ICP-MS ANALYSIS: ENHANCING HELIUM COLLISION AND REACTION CELL MODES. **R. Bastian Georg** & Clint Walker. Agilent Technologies Canada, 6705 Millcreek Dr., Unit 5, Mississauga, L5N 5M4, Ontario, Canada (bastian.georg@agilent.com)

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

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

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

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