ONLINE EVENT

DR. ANNA VEDDA
DR. ALEXANDER J. STIRK
KEYNOTE SPEAKERS

OCTOBER 30th
REGISTRATION DEADLINE

www.concordia.ca/CBGRC
INFORMATION

TABLE OF CONTENTS

WELCOME NOTE // LETTRE DE BIENVENUE

Dear friends and colleagues,

We are very excited to welcome everyone to the 23rd annual Chemistry and Biochemistry Graduate Research Conference. The goal of the CBGRC has always been to gather graduate students, professors and industry representatives in a comforting environment. While this year has been especially difficult for everyone in the scientific community, the CBGRC celebrates the achievements we've made despite numerous obstacles. Though we have taken the conference online, we hope to provide an amazing at-home experience and to inspire your research to new heights. We would like to thank everyone for your help in making the CBGRC a continued success, and we look forward to listening to your presentations.

The CBGRC Organizing Committee

Cher(e)s ami(e)s et collègues,

Nous sommes très heureux d'accueillir tout le monde à la 23e Conférence annuelle sur la Recherche aux Cycles Supérieurs en Chimie et Biochimie. Le but de la CRCSCB est de rassembler les étudiants aux cycles supérieurs, les professeurs et les représentants de l'industrie dans un environnement réconfortant. Bien que cette année ait été particulièrement difficile pour tous les membres de la communauté scientifique, la CRCSCB célèbre les réalisations que nous avons accomplies malgré de nombreux obstacles. Nous ayons mis la conférence en ligne, mais nous espérons de t'offrir une expérience incroyable à la maison et d'inspirer votre recherche vers de nouveaux sommets. Nous vous remercions pour votre aide à faire la CRCSCB un succès continu, et nous avons hâte d'écouter vos présentations.

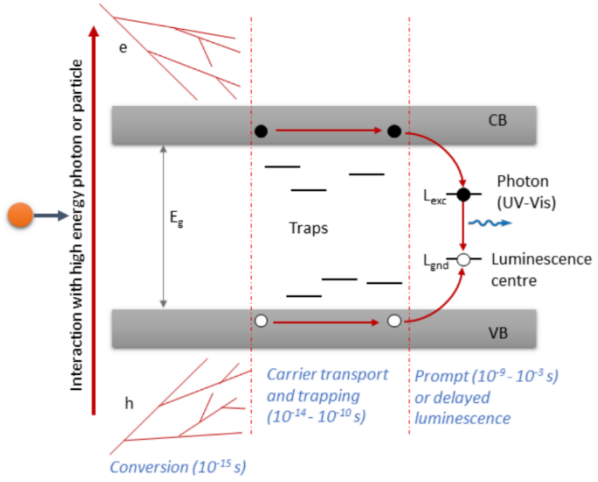
Le Comité Organisateur de la CRCSCB

MORNING KEYNOTE SPEAKER – DR. ANNA VEDDA // 10:00 AM EST

ABOUT DR. ANNA VEDDA

Anna Vedda is full professor of Experimental Physics of Matter at the Department of Materials Science of the University of Milano-Bicocca. Her principal fields of research concern the functional properties of scintillating materials for medical applications and high energy physics experiments. During her career, she has investigated various types of pure and rare-earth doped systems like scintillating glasses, crystals, optical ceramics, and nanomaterials. She published more than 260 papers in international journals and referred international conference proceedings, one book, and she is co-author of one patent. At present her publications received 5900 citations and her h-factor is 38 (Source: Scopus). She acts as referee of several scientific journals and was responsible of both national and international (H2020, NATO, INTAS) research projects. A.V. is member of the scientific committees of ICDIM/EURODIM, LUMDETR, and "SiO2, Advanced Dielectrics and Related Devices" international conference series. She is member of the Academic Senate, deputy director of the Department of Materials Science and member of the Department board. She is also member of the scientific board of the Doctorate in Materials Science and Nanotechnology of the University of Milano-Bicocca. Moreover, A.V. serves as delegate of the University, core partner in the Knowledge Innovation Community on Raw Materials (KIC-RM) supported by the European Institute of Innovation and Technology (EIT); she is also a member of the KIC-RM International Education Committee.

ABSTRACT: ROLE OF RARE-EARTH IONS IN SCINTILLATING MATERIALS



Scintillators are materials able to efficiently convert the energy deposited by high energy photons or ionizing particles into a great number of photons in the visible or near ultraviolet range, that can be detected by conventional photodetectors. They are extensively used for various applications, like for example medical diagnostics, high energy physics experiments, security, or industrial controls. The investigations on scintillators started soon after the discovery of X-rays, and faced a notable improvement especially in the last decades with the advent of several novel materials [1]. Among inorganic materials, fluorides, chlorides, bromides, iodides, and oxides single crystals are being developed. In several cases rare earth ions (RE) are present, either as lattice constituents and, especially, as luminescent activators. RE-doped scintillating glasses and, more recently, optical ceramics are also investigated. Indeed, RE ions present electronic configurations that permit a rich variety of radiative transitions and make them useful for different optical applications, including scintillation. For the purpose of scintillation, the allowed 5d-4f radiative transition is particularly useful, due to its high quantum efficiency and fast decay in the 10^{-7}-10^{-8} s time scale. For this reason, Ce^{3+}, Pr^{3+} or Eu^{2+}, featuring 5d-4f transitions in the visible or near ultraviolet in most host materials, are frequently considered. Scintillation is a complex process involving i) the absorption of the primary radiation beam and the production of a great number of free carriers; ii) the diffusion of free carriers and their transport to the luminescent centers, like RE ions; and finally, iii) the radiative recombination of electron-hole pairs giving rise to photon emission (Fig. 1). Good ionizing radiation absorption, radiation resistance, efficient and fast response are crucial properties to be considered for the engineering of a novel scintillator material. This lecture will first describe the scintillation phenomenon and the parameters that characterize scintillator material performances; the role of RE ions is then introduced, providing several examples in which RE are present, like lutetium/yttrium silicate single crystals [2], silicate glasses [3], complex garnet optical ceramics [4]; the particular case of PbWO4, the material used in the Large Hadron Collider at CERN for the discovery of Higgs Boson and in which RE ions were used as optically inactive dopants, is also presented [5]. A look to future scintillator needs is finally presented, especially concerning positron emission tomography medical diagnostics apparatuses in which a time response faster than 1 ns will be required; possible solutions involving RE doped materials, or nanocomposites made by luminescent nanoparticles embedded in a polymeric material [6] are outlined.

[1] C. Dujardin et al., "Needs, trends and advances in inorganic scintillators", IEEE TNS 65, 1977 (2018). [2] S. Blahuta et al., "Evidences and consequences of Ce in LYSO:Ce,Ca and LYSO:Ce,Mg Single Crystals for Medical Imaging Applications", IEEE TNS 60, 3134 (2013). [3] F. Cova et al., "Dual Cherenkov and scintillation response to high-energy electrons of rare-earth doped silica fibers" Phys. Rev. Appl., 11, 024036 (2019). [4] S. Liu et al., "Towards bright and fast Lu3Al5O12:Ce,Mg optical ceramics scintillators", Adv. Opt. Mater 4, 731 (2016). Fig. 1: Simple scheme of the scintillation process [5] S. Baccaro et al., "Influence of La3+ - doping on radiation hardness characteristics of PbWO4", Phys. Stat. Sol. 160, R5 (1997). [6] M. Gandini et al., " Efficient, Fast and Reabsorption-free Perovskite-based Sensitized Plastic Scintillators", Nature Nanotechnology 15, 462 (2020).

AFTERNOON KEYNOTE SPEAKER – DR. ALEX J. STIRK // 3:30 PM EST

ABOUT DR. ALEX J. STIRK

Originally from Great Wyrley in the West Midlands of England, Alex completed his BSc in 2012 at the University of Leeds in West Yorkshire. During his time at Leeds he was bitten by the research bug while working with Prof. Terry P. Kee in the prebiotic chemistry of phosphorous. In a departure from seeking the origin of life, Alex moved to Windsor, Ontario in 2013 to study solid state molecular machines with Prof. Stephen J. Loeb at The University of Windsor. Graduating with his PhD in 2018, Alex was concerned about his employability considering his lack of publications, visa status, being a millennial, and lack of understanding when something should be taken seriously. Deciding to stay in Canada and after a wide employment search, Alex found employment as a crystallographer and solid-state chemist in the Research & Technology (R&T) group at Apotex Pharmachem Inc. in Brantford, Ontario. His research in the R&T group involves the solid-state chemistry of active pharmaceutical ingredients and their impact on generic pharmaceutical intellectual property. This work involves a multi-disciplinary team of crystallographers, crystal engineers, organic chemists, analytical chemists, chemical engineers and patent agents. Outside of pharmaceuticals Alex's research interests are the chemistry of mechanically interlocked molecules, metal-organic frameworks, topology, cocrystals and firing X-rays at things.

ABSTRACT: SO YOU'VE DECIDED TO MAKE A GENERIC PHARMACEUTICAL

Your boss comes to you one day, places a house brick in your hand and tells you to build a brick wall. They then proceed to give you many specifications that you must meet, however you must not copy previously built walls! What do you do? How do you place the bricks in order to build the wall so that it is still the same as other walls – but different?

The solid-state form of generic pharmaceuticals is like this situation. You can only use the brick that you are given (in this case a particular active pharmaceutical ingredient), yet you must be innovative and novel when compared to the brand pharmaceutical. When developing a new pharmaceutical solid form there are many pitfalls that one must avoid so that your form may eventually help patients in need. Some of these pitfalls are chemical in nature, while others legal. This talk outlines the dos and don'ts of crystal engineering a hypothetical successful generic pharmaceutical. The differences between industrial and academic concerns will also be discussed with an attitude towards helping both fields understand each other.

ROOM LINKS OVERVIEW AND CONFERENCE GUIDELINES

ROOM	LINK
1	https://concordia-ca.zoom.us/my/cbgrc1
2	https://concordia-ca.zoom.us/my/cbgrc2
3	https://concordia-ca.zoom.us/my/cbgrc3
4	https://concordia-ca.zoom.us/my/cbgrc4

CONFERENCE GUIDELINES:

- All presenters will be given screen sharing capabilities to present their visual aid during their presentation.
- Have a good quality microphone and station yourself in a room without background noises or echoes.
- Make sure your microphone is muted when you are listening to the presentations of your peers.
- While a webcam is strongly recommended for improved engagement with your audience, it is not mandatory.
- Ensure your name on Zoom and in your presentation is the same as the one used to register on the conferencereg.com/cbgrc website.
- ***Especially for shotgun presentations,*** include contact information in the form of an email address or QR code at the end of your presentation, in case someone in your audience would like to contact you for potential questions or discussions.
- ***Especially for shotgun presentations,*** it is recommended to attend the speed networking session after the shotgun presentations to communicate with your audience about possible questions or discussions.
- To be eligible for the Sponsor Raffle, you must attend the Zoom rooms of all sponsors during lunch and speak or chat with their representatives. Two Amazon gift cards for 50$ will be given for the raffle!
- Recording oral presentations and shotgun talks is strictly prohibited.
- All times are in EST.
- If you need help with anything, email cbgrc.concordia@gmail.com

SCHEDULE OVERVIEW

TIME (EST)	EVENT	LINKS
07:30 - 8:00	Welcome Announcement	CBGRC ROOM 1
08:00 - 09:45	Talk Session A	CBGRC ROOM 1 ORGANIC CHEMISTRY CBGRC ROOM 2 INORGANIC CHEMISTRY CBGRC ROOM 3 BIOCHEMISTRY CBGRC ROOM 4 PHYSICAL CHEMISTRY
10:00 – 11:00	Keynote Speaker – Dr. Anna Vedda	CBGRC ROOM 1
11:15 – 12:45	Talk Session B	CBGRC ROOM 1 ORGANIC CHEMISTRY CBGRC ROOM 2 INORGANIC CHEMISTRY CBGRC ROOM 3 BIOCHEMISTRY CBGRC ROOM 4 ANALYTICAL AND ENVIRONMENTAL CHEMISTRY
12:45 - 13:30	Lunch and Sponsor Presentations	CBGRC ROOM 1 Agilent Technologies SPONSOR ROOM CBGRC ROOM 2 Fisher Scientific SPONSOR ROOM
13:30 – 15:15	Talk Session C	CBGRC ROOM 1 MOLECULAR BIOLOGY CBGRC ROOM 2 NANO AND COMPUTATIONAL CHEMISTRY CBGRC ROOM 3 BIOCHEMISTRY CBGRC ROOM 4 ANALYTICAL AND CHEMICAL EDUCATION
15:30 – 16:30	Keynote Speaker – Dr. Alex Stirk	CBGRC ROOM 1
16:45 – 18:00	Shotgun Presentations	CBGRC ROOM 1 ANALYTICAL AND MOLECULAR BIOLOGY CBGRC ROOM 2 ENVIRONMENTAL, COMPUTATIONAL, NANOCHEMISTRY, CHEMICAL EDUCATION CBGRC ROOM 3 BIOCHEMISTRY CBGRC ROOM 4 ANALYTICAL AND INORGANIC CHEMISTRY
18:00 - 19:30	Break	CBGRC ROOM 1
19:30	Award Announcements	CBGRC ROOM 1

SCHEDULE // TALK SESSION A // 08:00 – 09:45 AM EST

ORGANIC CHEMISTRY — CBGRC ROOM 1

8:00 J. Allingham (Lakehead University): Design, Synthesis, and Characterization of a P.E.T. Diagnostic Agent
8:15 D. Campeau (University of Ottawa): The missing reactivity profile of ynamides8:30 C. Cruche
8:45 K. Muratov (University of Ottawa): Sterically hindered phosphines as ligands for selective gold catalysis
8:30 C. Cruché (Université de Montréal): Rational Design of Heteroleptic Copper-Based Complexes for Photocatalytic E→Z Isomerization of Alkenes.
9:00 E. Isbrandt (uOttawa): Use of P_2N_2 ligands to enable challenging nickel-catalyzed cross coupling reactions
9:15 A. Mansour (University of Ottawa): A gold-mediated nitrene-transfer/hydride shift cascade for the synthesis of polycyclic indoles
9:30 L. Mélin (UQAM): Development of First-in-Class Potent and Selective PB1 Inhibitors

INORGANIC CHEMISTRY — CBGRC ROOM 2

8:00 A. Melenbacher (The University of Western Ontario): The pathways and domain specificity of Cu(I) binding to human metallothionein 1A
8:15 L. Porto (University of Ottawa): Copper-mediated C-C Bond Formation of Organofluorine Compounds
8:30 M. Rupp (Université de Montréal): Homoleptic vs. heteroleptic design of methylated ruthenium(II) bis-terpyridine complexes
8:45 J. S. Dhindsa (The University of Western Ontario): Optoelectronic Properties of Molecular and Macromolecular Materials Derived from Boron Difluoride Formazanates and Platinum(II)-Acetylides
9:00 A. Yuan (University of Western Ontario): Metallothionein protects zinc enzyme carbonic anhydrase from cadmium toxicity
9:15 F. Saraci (Concordia University): Exploring the crystalline phase changes of a Y_6-based MOF, CU-45

SCHEDULE // TALK SESSION A // 08:00 – 09:45 AM EST

BIOCHEMISTRY — CBGRC ROOM 3

8:00 Y. Ayotte (INRS - Armand-Frappier Santé Biotechnologie): Exposing Small-molecule Nano-entities By a Nuclear Magnetic Resonance Relaxation Assay
8:15 A. Bouchard (Université du Québec à Montréal): Novel molecular tools to understand the impact of SUMOylation on chosen cellular pathways
8:30 K. Chabi (Université du Québec à Montréal): Screening for reactive metabolites by LC-MS/MS using different trapping agents
8:45 S. Fonseca (Héma-Québec): Characterization of the antibacterial activity of a SiO_2 nanoparticle coating to prevent bacterial contamination in blood products
9:00 E. Garcia (University of Manitoba): Siramesine and lapatinib induce synergetic cell death in advanced prostate cancer cells
9:15 F. Hunter-Manseau (Université de Moncton): The Importance of the Mitochondrial Unfolded Protein Response in the Fruit Fly (***Drosophila melanogaster***) During Nutritional Stress
9:30 P. Jaouen (Université Laval): Membrane interaction of retinal proteins S100A1 and S100B

PHYSICAL CHEMISTRY — CBGRC ROOM 4

8:00 S. Bhagat (Concordia University): Electrospray deposition of conjugated polymers in ultra-high vacuum
8:15 H. Hase (Concordia University): P3HT:FxTCNQ – dopant strength and concentration are key to charge-transfer complex and ion-pair formation
8:30 C. Hennecker (McGill University): Multivalent Supramolecular Polymers
8:45 A. Laramée (Université de Montréal): Electrospinning of Highly Crystalline Polymers for Strongly Oriented Fibers
9:00 B. Martins de Lima (Concordia University): Analyzing the correlation between the polymer molecular weight and the chain conformation in the vicinity of a polymer/metal interface
9:15 F. Noël (Laval University): Influence of phospholipids on the membrane binding of the S100A16 protein in the presence of calcium
9:30 T. Spilfogel (McGill University): Uncovering the World of Halogen-Based Architectures in Solid-State Porphyrin Systems using the Cambridge Structural Database

SCHEDULE // TALK SESSION B // 11:15 AM – 12:30 PM EST

ORGANIC CHEMISTRY — CBGRC ROOM 1

11:15 R. Hernandez (Concordia University): Mechanochemical Synthesis of 3,5-Isoxazoles via 1,3-dipolarcycloaddition catalyzed by Cu/Al2O3 under Ball-Milling.
11:30 J. Vatté (Université de Montréal): Design, Synthesis and Biological Evaluation of Biguanide-PROTACs for Anticancer Therapeutics
11:45 D. Pal (Queens University): Regio- and Diastereoselective Rhodium-Catalyzed Allylic Substitution with Unstabilized Benzyl Nucleophiles
12:00 C. Buonomano (Concordia University): Use of Flow Chemistry for Decarboxylative Palladium-Catalyzed Cross-Coupling Reactions in the Synthesis of Heteroaromatics.
12:15 S. Wilson (Brock University): Synthesis of a Photocleavable Bolalipid for the study of Sec 14

INORGANIC CHEMISTRY — CBGRC ROOM 2

11:15 F. L. Buguis (The University of Western Ontario): Near-Infrared Boron Difluoride Formazanate Dyes
11:30 W. Leal (Concordia University): Conversion of Electrochemically Deposited Carbonates to Perovskites with Retention of Crystal Morphology
11:45 P. Donnarumma (Concordia University): Design, Synthetic Optimization, and Characterization of a new Rare-Earth Metal–Organic Framework
12:00 M. Esmaeili (University Of Guelph): UV-Induced Photoreactivity of β-***trans***-Cinnamic Acid
12:15 M. Hill (Ryerson University): Trapping PS_2: Synthesis and characterization of six stable dithioxophosphoranes derived from 2-acylmethyl-2-oxazolines.

SCHEDULE // TALK SESSION B // 11:15 AM – 12:30 PM EST

BIOCHEMISTRY — CBGRC ROOM 3

11:15 A. Kehinde (University of British Columbia): Variability and Diversity in Breadfruit (*Artocarpus altilis* and related hybrids) Starches
11:30 A. McAdorey (Brock University): Use of anion exchange chromatography to study nucleic acid polymorphism under native and denaturing conditions
11:45 J. McCain (McGill University): Photodynamic Inactivation of *E. coli* by a Theragnostic ROS-Activated Dormant Photosensitizer
12:00 J. Onyango (Western Michigan University): Identification of small-molecule miR-31 inhibitors through high throughput screening methods
12:15 S. Rajkumar (Goodman Cancer Research Centre, McGill University): Combination BRAF and MEK inhibition is effective in the treatment of *BRAF* non-p.V600 mutant melanomas with co-occurring *NF1* loss-of-function or oncogenic *NRAS* alterations.

ANALYTICAL AND ENVIRONMENTAL CHEMISTRY — CBGRC ROOM 4

11:15 Z. C. Guo (Thompson Rivers University): Characterization of Exchangeable and Total Recoverable Elements in the Soil Treated with Ash Residuals by Flame Atomic Absorption Spectrophotometry (FAAS) and Capillary Electrophoresis (CE)
11:30 J. Korner (University of Victoria): Artificial brain and intestinal "cells-on-a-chip" for drug permeability prediction
11:45 M. Lépine (Université du Québec à Montréal): Targeted analysis of the human tear proteome by LC-MS/MS
12:00 H. Tahmasbi (Concordia University): Systematic investigation of ion suppression and enhancement of polar compounds in liquid chromatography - electrospray high resolution mass spectrometry (LC-ESI HRMS)
12:15 A. Bain (McGill University): The refractive index of aqueous media: Considering solute concentration, wavelength and temperature
12:30 A. England (University of Guelph): Hydrodeoxygenation of 5-Carbon Sugar Alcohols to Diols via a Tandem Bicatalytic System

SCHEDULE // TALK SESSION C // 13:30 – 15:15 EST

MOLECULAR BIOLOGY — CBGRC ROOM 1

13:30 Y. Elmi (University of Ottawa): Revolutionary Phage Therapy
13:45 P. Ghosh (University of Manitoba): Proximity-dependent labeling with BioID to identify putative interacting partners of HYAL2, a cell surface hyaluronidase
14:00 I. Iasenza (Research Institute of the McGill University Health Centre, Montreal, QC, Canada; Division of Experimental Medicine, Department of Medicine, McGill University, Montreal, QC, Canada): High-throughput screen of primary human acute myeloid leukemia stem cells identifies novel anti-LSC compounds
14:15 N. Jiménez-Téllez (University of Calgary): Dexmedetomidine, a novel anesthetic with neuroprotective effects
14:30 S. Mehri (Windsor University): HLA Blockers for potentially treating Rheumatoid arthritis
14:45 H. T. Nguyen (Université de Moncton): Régulation transcriptionnelle de l'expression des cadhérines chez les cellules de sertoli du testicule
15:00 A. Simkovich (The University of Western Ontario): Two plants, one pathogen, a novel approach gives insight on Prune Dwarf Virus, an understudied virus

NANOCHEMISTRY AND COMPUTATIONAL CHEMISTRY — CBGRC ROOM 2

13:30 M. Kaur (Concordia University): Photostability of NIR 820 dye for the Sensitization of Upconverting Nanoparticles
13:45 S. McColman (Ryerson University): Tunable SARS-CoV-2 mimetic to study viral structure-function relationships
14:00 M. G. Rafique (McGill University): Functional 2D nanostructures via chemical and kinetic control of DNA-oligomer amphiphile self-assembly
14:15 Z. Singh (Concordia University): Donor-Chromophore-Acceptor Assembly Visible Light-Driven Oxidation of 1-Phenylpyrrolidine by a Heterogeneous Photoanode
14:30 G. Srivastava (Concordia University): Post-Synthesis Growth Mechanism of Lanthanide-doped Nanoparticles by Surface Modification
14:45 S. Liu (University of Guelph): Effects of solvated ions on electrochemical CO_2 reduction
15:00 R. V. Rakotoharisoa (University of Ottawa): Ensemble-based enzyme design can recapitulate the effects of laboratory directed evolution in silico Ensemble-based enzyme design can recapitulate the effects of laboratory directed evolution in silico

SCHEDULE // TALK SESSION C // 13:30 – 15:15 EST

BIOCHEMISTRY — CBGRC ROOM 3

13:30 D. Rocca (University of Lethbridge): snr30 in the Assembling Ribosome: Determining the Function of An Essential snoRNA in Ribosome Biogenesis
13:45 M. Silva (Memorial University): Phosphorylation-mediated opening of the mid-region of mammalian tropomyosin Tpm1.1 (α)
14:00 M. Simmons (McGill University): Shear-induced conformational transition in coiled-coiled protein fibers from freshwater mussels
14:15 K. Uggowitzer (McGill University): Connecting Function to Structure of Class II Lanthipeptide Synthetase using Extensive Kinetic Simulations and Tandem Mass Spectroscopy
14:30 E. Van Meter (Western Michigan University): High Throughput Screening for the Identification of Small Molecule Inhibitors of the pri-miRNA-18a-hnRNP A1 Interaction
14:45 N. Weerasinghe (McGill University): Exploring the conformational landscape of a lanthipeptide synthetase using native mass spectrometry
15:00 A. Yero (Université du Québec à Montréal): Dynamics of regulatory and effector CD8 T-cells in mesenteric lymph nodes and blood following very early ARV initiation in acute SIV-infected Rhesus Macaques

ANALYTICAL CHEMISTRY AND CHEMICAL EDUCATION — CBGRC ROOM 4

13:30 M. Mireault (Université du Québec à Montréal): Development of liquid chromatography-high resolution mass spectrometry method for human urine metabolomics
13:45 K. Ramsay (University of Victoria): The bottom-up synthesis of bespoke microfluidic prototissues
14:00 M. Mirabi (Concordia University): Evaluation of non-specific adsorption, solubility and ionization matrix effects for the determination of 12 mycotoxins in urine using dilute-and-shoot method
14:15 D. Yeung (University of Manitoba): Separation Orthogonality: How do you pair columns for 2D-LC MS/MS Proteomics?
14:30 J. Deng (University of Ottawa): Evaluating the impact of English language proficiency on chemistry students' abilities to construct scientific arguments
14:45 M. St-Onge Carle (University of Ottawa): Investigating how the delocalization learning outcomes are being enacted and achieved
15:00 A. Szozda (University of Ottawa): A pilot study: Investigating how undergraduate chemistry students engage in systems thinking in chemistry education and the impact of collaborative systems thinking tasks

SCHEDULE // SHOTGUN TALKS // 16:45 – 18:00 EST

CBGRC ROOM 1

P01 - J. Kaur (Dr B.R. Ambedkar National Institute of Technology, Jalandhar, India): Investigations on the Aggregation Behavior of an Ionic Liquid in Water + Carbohydrate Solutions – A Review
P02 - R. Kaur (Dr. B. R. Ambedkar National Institute of Technology Jalandhar Punjab India): A review on the aggregation study of an aqueous solution of hydrophilic ionic liquid in the presence of conventional surfactants
P03 - M. Keramatnejad (Concordia University): Characterization of Structured Films of Cholesteryl Oleate Using Surface Sensitive Techniques.
P04 - S. Charoughchi (Concordia university): Cyclopropene Core-based Molecules as Strong Electron Acceptors in Organic Semiconductors
M01 - V. Cerdeira (Université du Québec à Montréal): Novel neurodevelopmental genes in *C. elegans*
M02 - S. Chu (McGill University): Defining the bio-nano interactions of lanthanide-doped upconversion nanoparticles
M03 - M. Lefevre (Université du Québec à Montréal): Elucidating the gene regulatory network underlying gliogenesis in the enteric nervous system

CBGRC ROOM 2

E01 - B. Keenan (McGill University): Reconstructing Ancient Maya Population History Using Faecal Stanols
C01 - E. Cuierrier (Université de Montréal): The Exchange-Correlation Factor Model in Density Functional Theory
C02 - R. Dean (University of Ottawa): A Molecular Dynamics Investigation into the effect of ATP on Ryanodine Receptor 2
C03 - M. Miaro (University of Ottawa): Q277 stabilizes the cASIC1 desensitized state through electrostatic interactions and retards recovery
N01 - W. Copp (Concordia University): O^6-Alkylguanine DNA Alkyltransferase Mediated Disassembly of a DNA Tetrahedron
N02 – A. Clermont-Paquette (Concordia University): A promising new imaging tool for human cells: amine passivated fluorescent carbon dots
CE01 - N. Streja (University of Ottawa): A multi-institutional, longitudinal study investigating various curricular approaches to teaching and learning organic chemistry

SCHEDULE // SHOTGUN TALKS // 16:45 – 18:00 EST

CBGRC ROOM 3

B01 - N. Abraham (University of Guelph): Engineering the NADPH specificity of DepB, a novel aldo-keto reductase involved in the detoxification of the agroeconomic mycotoxin deoxynivalenol (DON).
B02 - M. Belleperche (McGill University): Fluorescent structure-switching aptamers for real-time monitoring of ROS activity
B03 - N. González Suárez (Université du Québec à Montréal): Targeting adipogenesis with green tea derived catechins: An impact on the paracrine regulation of triple-negative breast cancer progression
B04 - S. Hamry (McGill University): Genome mining of Novel Class II Lanthipeptides from Actinomycetes
B05 - S. Jmii (UQAM Sciences): Structural characterization of SUMOylation events in ***Arabidopsis thaliana,*** a post-translational modification involved in environmental stress response
B06 - S. Saran (University of Saskatchewan): B-factor analysis suggests that *L*-lysine and *R, R*-bisLysine allosterically inhibit *Cj*.DHDPS Enzyme by decreasing its protein dynamics
B07 - J. Vanloon (Brock University): Circular dichroism study of DNA conformations at biologically relevant concentrations
B08 - L. Wang (Department of Pharmacology and Therapeutics, McGill University): Drug-derived DNA damage as a predictive biomarker in personalized medicine

CBGRC ROOM 4

A01 - O. Ousji (Université du Québec à Montréal): *In vitro* metabolism of Epigallocatechin gallate (EGCG) analogs by LC-HRMS/MS
I01 - Y. Albkuri (University of Ottawa): Two for One: Reactivity of Nickel SNS Bis(thiolate) and its Ni(N_2S_2) Isomer
I02 - L. Cottin (Université du Quebec à Trois-Rivières): X-Ray Diffraction Structures of Bulky *N,N'*-Disubstituted Aryl Amidines : the *N,N'*-Bis(2,6-diisopropylphenyl)-4-pyridylamidine
I03 - M. Elsby (University of Ottawa): Design of Base Metal Catalysts for Bifunctional Catalysis Utilizing Biomimetic SNS Ligands
I04 - S. Norouziyanlakvan (University of Ottawa): Electrocatalytic Generation of H2 from Neutral Water in Acetonitrile Using Ni(II)"PN3P" Pincer Supported Complexes with Ligand Assistance
I05 - J. Ricardo-Noordberg (Concordia University): Functionalization of Semiconductor Surfaces Towards Solar Energy Conversion: Morphological Control, and Photonic Crystals
I06 - H. de Aguiar Bicalho (Concordia University): Mixed-linker metal–organic frameworks for the removal of organic pollutants from water

Characterization of Exchangeable and Total Recoverable Elements in the Soil Treated with Ash Residuals by Flame Atomic Absorption Spectrophotometry (FAAS) and Capillary Electrophoresis (CE)

Z. C. Guo[1*], K. Donkor[1], G. Whitworth[1], J. Barisher[2], T. Asingo[1]
[1]Thompson Rivers University, [2]Louisiana-Pacific Canada Ltd.

Hog fuel is the by-product of an engineered wood facility. Hog fuel is used as an input to biomass power plants ash residuals are produced as a waste by-product. Even though the ash residuals are high in nutrients, they are considered as a waste product, and normally stored at a landfill. In order to prevent the ash residuals from building up in landfills and creating an environmental hazard, and to reduce costs, the potential use of ash residuals as a fertilizer in agriculture are evaluated, which is done in collaboration with a biomass company and an agricultural research company based in B.C. In the study, ash residuals are agriculturally pH-treated with elemental sulfur and then applied to testing fields as a fertilizer every spring. The quantities of macro minerals, trace minerals and toxic elements in the fields are monitored throughout the growing seasons between 2018 and 2019. Mehlich-3 extraction and wet digestion are applied for preparing samples to quantify the exchangeable and total recoverable elements, respectively, in soil samples by using flame atomic absorption spectrometry (FAAS) and capillary electrophoresis (CE). Based on the changes of these elements, the impact of using ash residuals as a fertilizer in agriculture is evaluated.

Artificial brain and intestinal "cells-on-a-chip" for drug permeability prediction

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Over 90% of drug candidates fail between the earliest stages of development and the final commercial product. Development of new methodologies of predicting pharmacokinetic parameters of drug candidates, such as permeability in specific human tissues, is vital to the improvement of efficiency of these research phases. We propose that using droplet interface bilayers (DIBs) as a new type of pharmacokinetic compartment model on a microfluidic platform will avoid many of the difficulties and drawbacks of the methods currently in use. We create artificial brain and small intestine "cells-on-a-chip" for permeability prediction in the early stages of the drug development process. Using a microfluidic platform paired with a fast-response pressure pump to create and guide ~0.5nL aqueous microdroplets in a phospholipid-oil bulk phase, model cell membranes form at the droplet-droplet interfaces, creating acceptor and donor compartments separated by a biomimetic lipid bilayer. We report membrane permeability results from human small intestine and blood-brain barrier DIB assays using the xanthene fluorophores fluorescein and calcein. We also report preliminary findings tagging amine drugs *in situ* using fluorescamine; fluorescence detection is enabled as the drug diffuses across the biomimetic bilayer, yielding concentration information which can be converted into the apparent permeability coefficient P_{app}.

Targeted analysis of the human tear proteome by LC-MS/MS

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Eye diseases are widespread in the population, and can cause a multitude of side effects. Proteins in tears have an important role in eye health, and have been shown previously to correlate with some diseases. The comparative analysis of proteins from tears could identify biomarker proteins for many ophthalmological diseases. We are currently developing a robust and sensitive method for profiling tear proteins, from healthy volunteers. Tear samples were collected on tear strips and tryptic digestion was performed. Different LC-MS/MS methods have been compared including microflow and regular flow HPLC as well as incorporating pre-fractionation of peptides to increase proteomic coverage. We have compiled a database of all proteins found in tears from healthy volunteers. We have detected over 730 proteins in tears, within 1% false discovery rate criteria. We are currently building a targeted multiple reaction monitoring (LC-MRM) based

method to quantify these proteins in tear digests. A combination of data-dependent and data-independent (SWATH) experiments has been used to build this quantitative method from healthy volunteers as well as patients with different eye diseases. The optimized method will be employed to study several eye-related pathologies, including certain rare eye diseases and corneal transplant rejection.

Evaluation of non-specific adsorption, solubility and ionization matrix effects for the determination of 12 mycotoxins in urine using dilute-and-shoot method

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Mycotoxins are secondary metabolites produced by filamentous fungi, and they can cause severe toxic effects in humans. The goal of this study is to develop an LC-HRMS method for the detection of citrinin, ochratoxin A, ochratoxin alpha, fumonisins B1 and B2, alternariol, alternariol monomethyl ether, beauvericin, enniatins A1, A, B and B1 in urine. Initial method development focused on "dilute-and-shoot" method to permit high sample throughput. Two different solvents, 60% methanol (v/v) with 1% formic acid, and 4.5% acetonitrile with 0.9% formic acid (v/v) as recommended in literature were compared to investigate the influence of analyte solubility on 72hr autosampler stability. The results demonstrated that enniatins and beauvericin have low solubility in high aqueous solvent with 70-98% decrease in signal intensity. Additionally, non-specific adsorption in plastic HPLC inserts and glass vials was tested. The signal intensity for plastic inserts was higher in both solvents, indicating non-specific adsorption to glass. Furthermore, different dilution factors (1:10, 1:15, and 1:20) were tested for ten individual lots of urine of varying hydration status. 1:20 dilution factor can improve matrix-effect for urine samples containing high level of creatinine.

Development of liquid chromatography-high resolution mass spectrometry method for human urine metabolomics

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Metabolomics has grown in importance over recent years, and aims at quantifying metabolic changes from a biological sample by measuring small molecule metabolites. Urine is commonly used in metabolomics due to his wide range of metabolites and his accessibility. An unusual variation of these metabolites can predict changes occurring from dietary changes, environmental contaminants or pharmaceuticals, as well as serve as potential biomarkers of certain metabolic diseases. We have been working towards developing an LC-MS/MS method to cover the wide range of metabolites present in urine samples. For this, we compared four chromatographic columns and different sample extraction procedures, including protein precipitation, sample dilution and solid-phase extraction. Our preliminary results showed that two complementary columns covered a large number of urinary metabolites. For the sample preparation, protein precipitation using methanol and simple dilution of urine showed the best results. In the near future, we will analyze 400 urine samples to study the variability in metabolites in a healthy population from different backgrounds and dietary habits.

The bottom-up synthesis of bespoke microfluidic prototissues

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The ability to build biological tissues from their most fundamental chemical constituents has long been a subject of interest in the evolutionary, medical and materials science communities. When these chemical constituents become a primordial form of life they are referred to as protocells. A step up from protocells are prototissues; a combination of protocells that perform a collaborative function. Here we have outlined a cutting-edge approach for the bottom-up creation of prototissues using microfluidic technology. Our research group has developed a microfluidic platform for the creation of multicompartmental droplets, which is particularly advantageous for the biochemical engineering of artificial cells and tissues as it allows us to achieve a level of precision, consistency and accuracy that cannot be accessed using conventional methods such as centrifugation or manual shaking. Some of these inner droplets are tagged with an azide-conjugated bovine serum albumin nanoconjugate and the others with a bicyclononyne nanoconjugate. The unique geometric

configurations and thermoresponsivities of these interlinked prototissues were further analyzed. Overall, our microfluidic methodology opens up a unique route to the bottom-up fabrication of artificial tissue-like materials capable of collective behaviours and addresses an important gap in the fundamentals of the prototissue chemistry.

Systematic investigation of ion suppression and enhancement of polar compounds in liquid chromatography - electrospray high-resolution mass spectrometry (LC-ESI HRMS)

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Ion suppression and enhancement are well-known issues in ESI, but surprisingly very little fundamental information is available to predict which compounds and compound classes may be more prone to ionization matrix effects. To address this gap, this study evaluated matrix effects of well-defined mixtures of co-eluting metabolites: amino acids, organic acids and vitamin B metabolites. Fast C18 LC was used to co-elute together the desired pairs, and negative ESI modes were investigated when applicable. HRMS analysis was performed using Agilent 6545 QTOF equipped with Jetstream ESI source. This study reveals that in negative mode of ESI, some organic acids such as succinic acid were suppressed by all co-eluting compounds including α-ketoglutaric, citric and nicotinic acids. This likely indicates competition between analytes for the limited amount of charge. α-ketoglutaric acid was enhanced by succinic acid. This may be attributed to an increase the amount of charge on the surface of the droplet thus increasing efficiency of ionization and causing ion enhancement in some cases. Some amino acids such as glutamic acid were suppressed by organic acids like malic acid. Proline was suppressed by glutamic acid but not *vice versa*. This indicates that this is not a polarity-driven mechanism.

Separation Orthogonality: How do you pair columns for 2D-LC MS/MS Proteomics?

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University of Manitoba

In the ever-expanding field of proteomics, 2D-LC MS/MS has been a staple for digging deeper in the analysis of complex proteomes. Current standards include pairing: Strong-Anion Exchange (SAX) with Reverse Phase (RP), pH 10 RP with pH 4.5 RP, Hydrophilic Interaction Liquid Chromatography (HILIC) with RP, but how do we know which has the best identifications? From our decades of experience in modeling predictive algorithms for chromatographic columns with SSRCalc, we set out to establish a standard for which proteomics practitioners can refer to for their sample preparation in 2D-LC MS/MS. Assessing 16 different chromatographic columns and their pairing against RP, we quantitative measure the orthogonality between different columns to understand their differences in separation mechanisms. Does higher orthogonality lead to larger identification?

The refractive index of aqueous media: Considering solute concentration, wavelength and temperature

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From oceans, lakes and rivers to the aerosol suspended in our atmosphere, aqueous media are abundant in our environment. These systems contain water, but also inorganic salts and acids as well as dissolved organics. Understanding the optical properties of aqueous systems is important in many applications, including determining radiative forcing for climate calculations, remote satellite sensing, analysis and simulation of underwater light fields, and underwater photography missions. The optical properties of pure water are known with high precision, but there are few examples of concentration-dependent refractive index parameterizations for inorganic and organic solutes. In many cases, we are interested in how these aqueous systems interact with solar radiation and dispersion must be also considered. Furthermore, aqueous systems such as aerosol and sea ice brine may exist in supersaturated and/or supercooled states. Here, I will discuss single particle measurements of the refractive index of aqueous particles, which allow access to the full range of environmental concentrations including these metastable states, and a refractive index model, which allows for the calculation of the refractive index of aqueous media as a function of solute concentration, wavelength and temperature.

Hydrodeoxygenation of 5-Carbon Sugar Alcohols to Diols via a Tandem Bicatalytic System

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As the ramifications of petrochemical production have become apparent, a strong interest in the development of biomass-based processes for commodity chemical production has formed. Among the most coveted of biomass-derived products are the alpha-omega diols, which are drop-in monomers for polyesters and polyurethanes, and convenient precursors to polyamide monomers. The most common substrates investigated for diol production on the laboratory scale are furanics such as furfural, as the chief alternatives, sugar alcohols, have little to no solubility in organic solvents. However, significant challenges in preventing self-reactivity of biomass-derived furanic substrates has hindered the industrial implementation of biomass conversion processes. To mitigate these challenges our work has focused on acetylated sugar alcohols, which have favourable self-reactivity and solubility properties. Hydrodeoxygenation is achieved via a tandem Lewis acid and hydrogenating metal catalyst system. Various Lewis acids have been investigated via time-series reactions to optimize yield of 1,4 and 1,5-pentandiol.

Near-Infrared Boron Difluoride Formazanate Dyes

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Western University

Chromophores that exhibit optical properties, such as absorbance and photoluminescence, in the far-red and near-infrared (NIR) spectral regions have garnered significant attention. These dyes are sought after due to their utility in material science and bioimaging applications, leading to the continuous search for new architectures. Typical challenges that need to be overcome in this research space are long synthetic routes and expensive starting materials. In our most recent efforts, the addition of tertiary amine substituents into the BF_2-formazanate architecture yielded chromophores with NIR optical properties similar to dyes with more complex structures. Cyclic voltammetry experiments revealed multiple reversible redox waves linked to the interplay between the tertiary amine and formazanate moieties. Density-functional calculations revealed the electronic transitions to be $\pi \rightarrow \pi^*$ type between strongly delocalized molecular orbitals with an exception of one dye exhibiting charge-transfer type transitions. The insights gained in this work serve as a platform for next-generation BF_2-formazanate dyes and demonstrate the feasibility of relatively simple π-conjugated systems for NIR applications.

Optoelectronic Properties of Molecular and Macromolecular Materials Derived from Boron Difluoride Formazanates and Platinum(II)-Acetylides

J. S. Dhindsa*, R. R. Maar, S. M. Barbon, J. B. Gilroy
Western University

Organic π-conjugated molecular and polymeric materials exhibit sought after optical and electronic properties due to the delocalization of π-electrons within their frameworks and are often semiconducting. This leads to their use in a variety of organic electronics such as light emitting diodes, lasers, photovoltaic devices, memory devices, etc. Incorporating platinum(II) into the main chain of these systems is known to afford a variety of advantageous properties such as photoluminescence, redox activity, and optoelectronic properties. The general structure for platinum polyynes is a linear backbone comprised of the platinum(II) center, supported by neutral phosphine ligands, and a spacer group. Herein, we introduce a readily accessible conjugated polymer and several molecular compounds that couple electron-poor boron difluoride formazanate spacers and electron-rich platinum(II)-acetylide subunits as promising candidates for use in organic electronics. We have also demonstrated advantageous thin film forming properties and stepwise, controlled chemical reduction of the polymer.

Design, Synthetic Optimization, and Characterization of a new Rare-Earth Metal–Organic Framework

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Concordia University

Metal–organic frameworks (MOFs) are a family of structurally diverse, self-assembled materials built up from inorganic and organic units. The most prominent feature of MOFs is the existence of permanent pores in their structures, which in turn makes them very attractive materials for wide ranging applications, from gas adsorption to photocatalysis. Hexanuclear rare-earth (RE) clusters offer unique opportunities as MOF nodes and open the door towards the synthesis of a new class of functional RE-MOFs. Using linear linkers, it is possible to use these clusters to build a new series of RE-MOFs related to the archetypical UiO-66, originally made out of Zr-hexanuclear clusters and terephthalic acid linkers. The design and optimization of synthetic protocols for MOFs is key to obtaining pure and high-quality materials. There are many parameters that govern the formation of a specific MOF and all of them can be impactful in the final result. As such, it can be very challenging to understand concretely how the different parameters play out in the MOF formation process. This presentation will discuss the design and optimization process for the synthesis of a novel RE-MOF, including the sensitivity of the process to various factors like time, temperature, and reaction medium.

UV-Induced Photoreactivity of β-*trans*-Cinnamic Acid

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trans-Cinnamic acid exists in three polymorphic forms that behave differently upon UV irradiation. In spite of the extensive photoreactivity studies on the α- and β-forms over the last six decades, there is still no full understanding of the cinnamic acid reactivity in the solid-state. We have investigated the photoreactivity of pure β-*trans*-cinnamic acid to be used as a model for our research on cocrystal systems. It is known that β-*trans*-cinnamic acid polymorph transforms into β-truxinic acid upon UV irradiation while the α-form produces α-truxillic acid. Our PXRD screening results suggest that the main product is formed with some side products, namely, benzoic acid, phenol, and α-truxillic acid. This preliminary hypothesis was then corroborated with our complementary NMR data. The observed side products have not been reported in the literature. The formation of the side products indicates that some molecules must have been oxidized or dissociated upon UV exposure. However, the mechanism of such reactions is not straightforward and needs to be studied further. Our studies also show the β-form is partially converted to α-form upon UV-irradiation. This finding suggests cinnamic acid is dynamic in the solid-state. We will present the kinetics of reaction along with other results.

Trapping PS_2: Synthesis and characterization of six stable dithioxophosphoranes derived from 2-acylmethyl-2-oxazolines.

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Ryerson University

Dithioxophosphoranes (DTPs) are an interesting class of compounds that are relatively unexplored in the chemical literature. They are defined by the structural fragment consisting of a pentavalent phosphorous center bonded to two terminal sulfurs and one or two other atoms that link to the rest of the molecule (*e.g.*, C, N, S). The paucity of research done on these compounds over the past 40 years is explained by their instability, low yields (<20%), and the numerous synthetic steps required for their production. However, in the course of the one-step thionation of 2-acylmethyl-2-oxazolines by phosphorous pentasulfide it was found that a PS_2 unit could be readily trapped to afford stable dithioxophospharane-oxazolines (Ditphoxes). This allowed for the synthesis and full characterization of six derivatives comprised of electron-withdrawing or donating groups in relatively high yield (32-78%). Additionally, it was found that addition of triethylamine to the reaction produces the intended thioketone-oxazolines that have great potential for the synthesis of transition-metal thiolate complexes. Overall, the research presented herein represents an exciting development in main-group coordination chemistry by greatly improving the availability of dithioxophospharanes for exploration of their untapped potential.

Conversion of Electrochemically Deposited Carbonates to Perovskites with Retention of Crystal Morphology

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Concordia University

Perovskite-based materials have been identified as candidates for use in many light-driven processes and devices. This stems from their intrinsic photophysical properties such as low exciton binding energy, long carrier diffusion length, and a tunable band gap. However, direct synthesis limits the morphologies that can be made, and control over the shape of perovskite crystallites may allow us to further tap into their potential. It has been reported that conversion of carbonate to perovskite microstructures can be achieved through ion-exchange reactions, with structure retention, though fundamental understanding of this process remains limited. Here we outline the electrochemical deposition of different morphologies of calcium carbonate on transparent conducting oxide substrates followed by *in situ* conversion of the resulting microstructures to all-inorganic perovskites (of the stoichiometry ABX_3) while retaining the overall microstructure. After electrochemical deposition, the microstructures are exposed to a concentrated solution of lead nitrate to enable cation exchange. Subsequent ion exchange reactions lead to the conversion to the expected perovskite. Organic capping groups can be incorporated in the conversion process to passivate the surface, improving the perovskite stability and even improving defect tolerance. We are also working to investigate the conversion mechanism and the resulting photophysical properties of the microstructures.

The pathways and domain specificity of Cu(I) binding to human metallothionein 1A

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Copper redox chemistry is key to many enzymes. However, this redox chemistry can lead to reactive oxygen species if uncontrolled, which can be fatal to the cell. Cellular proteins bind metals tightly to alleviate toxicity. Metallothionein (MT), a protein with 20 cysteines, is involved in homeostatic control of Zn(II) and Cu(I) and binds metals in metal-thiolate clusters. Electrospray ionization mass spectrometry (ESI-MS) has been used previously to identify a series of Cu(I)-MT species which have 6, 10, and 13 Cu(I), however it is unclear what individual clusters make up these species and which domain of MT the individual clusters form in. Detailed native ESI-MS studies with the isolated domain fragments of MT have been used to determine the clusters that form the key species in the full protein. Competition studies with the fragments were used to identify the domain preference of Cu(I) binding as well as the relative stabilities of the clusters. Extensive simulations of the Cu(I) species formed provided the relative binding constants for the 20 Cu(I) ions bound to MT.

Copper-mediated C-C Bond Formation of Organofluorine Compounds

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Fluorine's high electronegativity and small size bestows unique and advantageous physical and chemical effects on its compounds. The inclusion of fluorine and fluoroalkyl groups into organic molecules enhances the bioactivity and modulates pharmacokinetics, thus representing an important class of targets for medicinal chemistry. In 2018, Baker et al. synthesized LnCu-CF(CF3)2 (Cu-HFIP) reagents by insertion of hexafluoropropene, F2C=CF(CF3), into (PPh3)3Cu-F. Using phenanthroline as ancillary ligand, they demonstrated efficient transfer of the HFIP group to aroyl chlorides [1]. In this work, we describe the generation of a new RF group [-CF(OCF3) (CF2H)] from reaction of F2C=CF(OCF3) with [(PPh3)CuH]6 (Stryker`s reagent) and PPh3. We isolated three different complexes with one N-heterocyclic carbene (NHC), two PPh3 and three P(OEt)3 ligands and only that with NHC was able to transfer the RF to aroyl chlorides. Attempts using bipy or DMSO as a ligand (1 equivalent) yielded an expansion of the organic electrophile substrate scope (to aryl iodides, for example). We are currently working with a computational chemistry collaborator to better understand the ligand dependence on transfer efficiency of this RF group.

Homoleptic vs. heteroleptic design of methylated ruthenium(II) bis-terpyridine complexes

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In this study, we investigate the impact of *N*-methylation on the electronic and photophysical properties of both homoleptic and heteroleptic ruthenium(II) bis-terpyridine complexes based on the recently reported ligand 4'-(4-bromophenyl)-4,4''':4'',4''''-dipyridinyl-2,2':6',2''-terpyridine (Bipytpy), with pyridine substituents in the 4- and 4''-position. The first reduction of the methylated complexes takes place at the pyridinium site and is observed as multi-electron process. Following *N*-methylation, the complexes exhibit higher luminescence quantum yields and longer excited-state lifetimes. Interestingly, the homoleptic complexes show an excitation wavelength-dependent emission behavior, related to the co-existence of multiple emissive metal-to-ligand charge-transfer states, as shown by TD-DFT calculations. Furthermore, based on their improved photophysical properties, these complexes are tested as photosensitizers for photocatalytic hydrogen production, as complex $[Ru(Bipytpy)(Tolyltpy)](PF_6)_2$ (Tolyltpy: 4'-tolyl-2,2':6,2'-terpyridine) was recently shown to be active and highly stable under photocatalytic conditions. However, loss of the methyl groups under photocatalytic conditions prevent the observation of the expected enhanced photocatalytic activity.

Exploring the crystalline phase changes of a Y_6-based MOF, CU-45

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Over recent years, metal–organic frameworks (MOFs) have emerged as a class of hybrid porous materials constructed from inorganic and organic building units that form often-crystalline, robust, and multi-dimensional materials with high surface areas. Recently, MOFs constructed with rare-earth (RE) elements, including scandium, yttrium and the series of fifteen lanthanides, have emerged as a fascinating family of MOFs. Owing to the high coordination numbers and distinct electronic and optical properties, RE-MOFs demonstrate complex structures and topologies that display diverse features and functionality. Herein, we present the formation of CU-45 (CU = Concordia University), comprised of Y-nodes, bridged by tritopic organic linkers. CU-45 undergoes a crystalline-to-crystalline phase transformation in response to thermal energy, varying solvent polarity and pH, and pressure. The synthesis, characterization, and details of the phase transformation of CU-45 will be discussed.

Metallothionein protects zinc enzyme carbonic anhydrase from cadmium toxicity

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Western University

Metallothioneins (MTs) are a physiologically vital protein family for essential metal homeostasis and heavy metal detoxification. Using its twenty cysteines, MTs protect the proteome by sequestering heavy metals into thermodynamically stable metal (M) thiolate (S_{Cys}) structures, $M_4(S_{Cys})_{11}$ and $M_3(S_{Cys})_9$, only when fully metalated. Although heavy metal cadmium (Cd) metalation of MT is well-characterized, it has not been studied extensively in solution with other metalloproteins such as carbonic anhydrase (CA). Using stopped-flow kinetics and electrospray ionization mass spectrometry, we quantified Cd^{2+} binding of MT in the presence and absence of CA at both physiological pH (7.4) and low pH (5) using known its known binding constant to CA. We observed the association between apo-MT and apo-CA, which enhances the formation of the protective mode of MT, where $Cd_4(S_{Cys})_{11}$-clusters form at much lower concentration levels. This protein association affects the Cd^{2+} metalation rates of MT. The data support the physiological role of MTs as protectors of the metalloproteome from the toxic effects of Cd^{2+} through stable sequestration of the metal prior to Cd^{2+} exposure to other metalloproteins. Thank you to NSERC Canada for supporting this research through the Discovery Grant, CGS-M, and PGS-D scholarships.

ABSTRACTS // ORGANIC CHEMISTRY ORAL PRESENTATIONS

Design, Synthesis, and Characterization of a P.E.T. Diagnostic Agent

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Concussions are an increasingly significant issue, especially in the sports community. Despite this fact, there is currently no single standard, objective criterion for diagnosing mild traumatic brain injuries, like concussions. The diagnostics of concussions are difficult because their symptoms are often observed in the absence of significant structural damage making neuroimaging techniques such as computerized tomography (CT) and magnetic resonance imaging (MRI) exceedingly difficult to use to identify their presence. An objective test with high sensitivity and specificity for concussions would provide a substantial advance in concussion diagnostics, which can help in the prognosis, treatment, and medical decision-making regarding the disorder. This research is conducted to fill the void in concussion diagnostic techniques by synthesizing a small molecule 18F-radiotracer capable of binding to a biomarker of neuronal trauma, thus allowing for the imaging of its upregulation using a PET scanner. I have employed virtual screening to develop a radiotracer for a biomarker. To prove the binding of my tracer to the biomarker *in vitro*, I employed enzyme-linked immunosorbent assay (ELISA); followed by *in vivo* analysis utilizing small animal imaging, with mice as a model, administering concussions using high intensity focused ultrasound (HIFU) and imaging the mice using a microPET scanner.

Use of Flow Chemistry for Decarboxylative Palladium-Catalyzed Cross-Coupling Reactions in the Synthesis of Heteroaromatics.

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Concordia University

The chemical industry plays a major role in the production of chemicals; however, it often results in pollution and the release of toxic contaminants. Green chemistry is the design of more environmentally friendly protocols that could reduce the generation of toxic substances. We decided to implement some aspects of this approach in our research for the synthesis of heteroaromatics using catalysis and flow chemistry. Heteroaromatics are key motifs present in many biologically active compounds. Their synthesis can be achieved via palladium-catalyzed cross-coupling reactions. Recently, decarboxylative cross-couplings have emerged as advantageous and greener alternatives to the classical methods reducing the production of harmful by-products. We have been investigating these cross-coupling methodologies for the past decades proving their usefulness. In order to increase the attractiveness of our methodologies for industrial applications, it is crucial to adapt them to new synthetic technologies. Continuous flow is a powerful technique using micro-tubes and small benchtop reactors. It offers advantages versus the batch processes commonly used in organic synthesis. The purpose of this research project is to apply the decarboxylative cross-coupling methodology developed by our group, and make it more efficient, versatile and cleaner using the flow chemistry techniques.

The missing reactivity profile of ynamides

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University of Ottawa

Ynamides, as relatively stable analogs of their parent ynamines, have proven to be useful building blocks in organic synthesis as attested by their use in an explosion of new synthetic methods over the past two decades. However, one unexpected yet crucial reactivity has been overlooked. We have discovered that ynamides can participate as the 4π-component in [3+2] cycloadditions with tethered alkynes to yield a variety of substituted pyrroles. Interestingly, this reaction occurs upon simple heating of a substrate solution without the need of any catalyst or reagent being present. Variously substituted ynamides and alkynes efficiently participate in this transformation, yielding a wide array of polycyclic fused pyrroles. On the basis of experimental and theoretical mechanistic studies, the reaction is proposed to proceed via a two-step cycloaddition-rearrangement sequence.

Rational Design of Heteroleptic Copper-Based Complexes for Photocatalytic E→Z Isomerization of Alkenes.

C. Cruché
Université de Montréal

Access of thermodynamically less stable Z-alkene through E→Z photocatalytic isomerization has gained an increased interest in the last decade. In most studies, Iridium-based photocatalysts or dyes are used, both lacking a rapid and easy design to find the ''sweet spot'' for an efficient isomerization. The Collins group has been studying libraries of heteroleptic copper complexes in different photocatalytic processes, in an effort to elucidate important structure/activity relationships. Results from the screening of the libraries and correlation of reactivity to photophysical properties in the E-to-Z isomerization of olefins will be presented.

Mechanochemical Synthesis of 3,5-Isoxazoles via 1,3-dipolarcycloaddition catalyzed by Cu/Al2O3 under Ball-Milling.

R. Hernandez*, P. Forgione
Concordia University

3,5-Isoxazoles are ubiquitous scaffold found in medicinal chemistry. Due to their high occurrence numerous synthetic protocols have been developed. 1,3-dipolar cycloadditions between an alkyne and a nitrile oxide is among the most common routes to efficiently access this motif. However, previous protocols suffer from important drawbacks such as high temperatures, long reaction times, use of oxidants, strong bases, or careful control of pH. Herein, we discuss a more environmentally benign protocol for the synthesis of 3,5-Isoxazoles via 1,3-dipolar cycloadditions from a broad library of alkynes and (E)-N-hydroxy-4-nitrobenzimidoyl chloride or ethyl (E)-2-chloro-2-(hydroxyimino)acetate catalyze by Cu/Al2O3 under Ball Milling Conditions in low to excellent yields, short reaction times, and less waste production than in solution base reactions.

Use of P_2N_2 ligands to enable challenging nickel-catalyzed cross coupling reactions

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University of Ottawa

The nickel-catalyzed 1,2-addition of organohalides to aldehydes is a well-established transformation for constructing C–C bonds. However, the vast majority of these reactions use a stoichiometric metal reductant to turn over the catalyst. We envisioned using simple, feedstock alcohols as reductants to couple aryl halides with aldehydes. Exhaustive screening found that traditional phosphines and related ligands were ineffective. In contrast, 1,5-diaza-3,7-diphosphacyclooctane (P_2N_2) ligands, previously unused in coupling chemistry, were discovered to be highly effective. Inexpensive alcohols can be used as stoichiometric reductants, enabling a broad scope of coupling partners. The synthesis and application of P_2N_2 ligands will be highlighted, providing an appealing alternative to existing coupling reactions.

A gold-mediated nitrene-transfer/hydride shift cascade for the synthesis of polycyclic indoles

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University of Ottawa

Catalysis by electrophilic gold complexes represents an increasingly powerful tool for the generation of molecular complexity and diversity. The Lewis acidic properties of electrophilic gold complexes provide an excellent opportunity for the efficient functionalization of carbon π-systems, particularly for alkynes and allenes. Gold complexes are also non-toxic and tolerant to water and oxygen, making them environmentally friendly. Developments in the field of gold(I) catalysis have provided a novel method for the formal transfer of a nitrene species onto a carbon π-system, where an α-imino gold carbene intermediate can be generated. Additionally, hydrogen-atom (H-atom) transfer under electrophilic gold(I) activation is a versatile method for the functionalization of organic molecules and can be viewed as a means of increasing their structural complexity. Herein, we report the design and development of a cascade process for the synthesis of polycyclic indole scaffolds using formal nitrene-transfer onto alkynes in combination with concomitant intramolecular H-atom transfer. Successful execution of this method will allow for the rapid generation of complex heterocyclic frameworks

which find applications in total synthesis, heterocyclic and medicinal chemistry. Reaction development, mechanistic details and the scope of the reaction will be discussed.

Development of First-in-Class Potent and Selective PB1 Inhibitors

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PB1 is a unique epigenetic reader that contains six distinct bromodomains. Although PB1 is hypothesized to act as the key nucleosome-recognition subunit of the chromatin remodeling complex PBAF, its exact role has not yet been elucidated due to the lack of potent and selective inhibitors. Knowing that somatic PB1 mutations occur in many cancers, including up to 50% of clear cell renal cell carcinomas (ccRCC), generating chemical probes that target different bromodomains within the protein would constitute highly valuable tools to elucidate the exact function and therapeutic pertinence of PB1 overall, and of each of its bromodomain. We report herein the development of quinazolinone derivatives which display strong affinity with various selectivity profile towards essential bromodomains 2, 4 and 5 of PB1 as assessed by DSF. Our lead compound binds to PB1(2), PB1(5) and SMARCA2 with K_d values of 110, 61 and 2100 nM respectively. This chemical probe potently targets PB1 with an unprecedented 34-fold selectivity profile over SMARCA2 and shows mild proliferation inhibition in cancer cell lines.

Sterically hindered phosphines as ligands for selective gold catalysis

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An increase of the steric hindrance around the gold center can lead to increased selectivity in gold-catalyzed reactions. A commonly employed strategy to access sterically constrained environments includes encapsulation of a gold atom in different macromolecular cages, but the advantages of these types of complexes are, however, usually impeded by their complex synthesis and poor atom economy. Our approach to addressing this problem relies on the employment of previously disregarded tris(biphenyl)phosphines as ligands, which, due to the linear geometry of the gold (I) complexes, creates an extremely sterically demanding environment around the gold atom. These ligands can be easily synthesized and allow potential modification using substituents of various steric and electronic nature. A series of gold-complexes with tris(biphenyl)phosphines were synthesized and their catalytic activity was evaluated in a series of benchmark skeletal rearrangements and hydration reactions. The developed catalysts showed exceptional selectivity and, in some cases, significantly higher reaction rates than classical phosphine- or NHC-based catalysts.

Regio- and Diastereoselective Rhodium-Catalyzed Allylic Substitution with Unstabilized Benzyl Nucleophiles

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The development of the transition metal-catalyzed allylic substitution reaction is dominated by “soft” stabilized nucleophiles, rather than “hard” unstabilized nucleophiles. This striking dichotomy can presumably be ascribed to the high reactivity of the "hard" nucleophiles, which often promotes unproductive reaction pathways. Although benzyl-motifs are ubiquitous in a number of bioactive molecules, the utilization of “hard” unstabilized benzyl organometallics is particularly challenging because of their decreased rate of reductive elimination, which is further exasperated by the formation of the Wurtz-type homocoupling product. This presentation will describe a highly regioselective allylic alkylation of “hard” benzylzinc nucleophiles in the presence of a rhodium(III) catalyst. Importantly, this method utilizes bench stable rhodium(III) chloride as a catalyst, in the absence of an exogenous ligand. The seminar will also outline the development of the diastereoselective variant, which permits both acyclic and cyclic allylic carbonates bearing a homoallylic stereocenter to undergo benzylation with high levels of diastereocontrol. Hence, this approach provides a rare example of 1,2-stereoinduction in transition metal-catalyzed allylic substitution.

Design, Synthesis and Biological Evaluation of Biguanide-PROTACs for Anticancer Therapeutics

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Recent studies on metformin's anti-cancerous properties led to a growing interest in the use of biguanides derivatives for cancer treatment and prevention. The mechanism of action of metformin on cancerous cells is still not fully understood and different hypotheses have been proposed in the literature. However, it is a well-known fact that its effect has only been observed for high doses of this drug. Our recent interest is to design and develop biguanide derivatives that will be more efficient than metformin when used in small amounts for the inhibition of the proliferation of cancer cells. Our strategy is to induce the degradation of the biguanide's target by using the Proteolysis-Targeting Chimera (PROTAC) technique. This approach consists in synthesizing bifunctional molecules containing a specific ubiquitin ligase's ligand and a biguanide moiety able to bind its target. This supramolecular system results in an ubiquitinated biguanide binding protein that can be recognized and degraded by the Ubiquitin-Proteasome System (UPS), while liberating the PROTAC-Biguanide, which is available for a new degradation cycle.

Synthesis of a Photocleavable Bolalipid for the study of Sec 14

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Phosphatidylinositol transfer proteins (PITPs) are nonenzymatic proteins that are ubiquitous in eukaryotes. Sec14 is a yeast PITP that has been shown to transfer phosphatidylinositol (PI) or phosphatidylcholine (PC) from the endoplasmic reticulum to the Golgi. Initially, it was believed that Sec14's role was that of a simple lipid transfer protein. However, it is believed that Sec14 may play a greater role than just shuttling PI and PC throughout the cell. There is genetic evidence to suggest that Sec14 may bind to membrane bound PI and presents it to the phosphatidylinositol 4-kinase (Pik1). Pik1 then phosphorylates PI to generate phosphatidylinositol-4-phosphate. This function of Sec14 can be verified by synthesizing a photocleavable bola-PI analogue. This photocleavable bola-PI will be designed to span an entire membrane, having one polar head group on each leaflet, and will be connected by a photocleavable diacid. It is believed that Sec14 will not be able to present this bola-PI to Pik1 for phosphorylation when it is in the un-cleaved state. Once cleaved, it is believed that Sec14 will resume normal activity and phosphorylation by Pik1 would resume. We report synthetic efforts towards a photocleavable group designed to cleave in the center of the bolalipid.

Photostability of NIR 820 dye for the Sensitization of Upconverting Nanoparticles

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Dye sensitization is one of the methods, employed to enhance upconversion luminescence of lanthanide upconverting nanoparticles (UCNPs). This method improves the photon harvesting capability of UCNPs and substantially enhancing their upconversion luminescence. However, limited photostability of NIR dyes makes such system unsuitable for prolonged use. In this project, we studied that IR 820 reacts with in-situ produced $^1O_2$, upon irradiation with 800 nm light, decomposing into oxindole and aldehyde products, making the NIR dye ill-suited for sensitization. Formation of degraded products have been confirmed by mass spectrometry. To circumvent this problem, IR 820 was functionalized with 4-nitrothiophenol, forming IR 820-NO_2, becoming more photostable than IR 820. Also, fluorescence of IR 820-NO_2 centered at 950 nm offers better overlap with the Yb^{3+} absorption band. IR 820 and IR 820-NO_2 dyes were individually grafted on oleate free $NaGdF_4$:Er^{3+},Yb^{3+}/ $NaGdF_4$:Yb^{3+}nanoparticles. Emission spectra of IR 820-NO_2-coated UCNPs showed improved enhancement of the Er^{3+}emissions, than IR 820-coated UCNPs. Kinetic studies of Er^{3+} $^4S_{3/2} \rightarrow {}^4I_{15/2}$ transition showed intense emissions and a longer duration time for IR 820-NO_2-coated UCNPs. Future work will be undertaken to measure the quantum yield of this the hybrid system.

Tunable SARS-CoV-2 mimetic to study viral structure-function relationships

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The SARS-CoV-2 virus, implicated in the COVID-19 pandemic, is a natural nanoparticle made of genetic material and proteins encapsulated by a membrane called the viral envelope. The spike glycoprotein, attached to the viral envelope, is involved in recognizing and binding host cells. Recent studies suggest that spatial distributions of the spike protein may influence viral immunogenicity. The aim of this study is to create the first ever tunable simulated SARS-CoV-2 virus, or viral mimetic (VM), consisting of viral proteins inserted in a liposomal nanoparticle. This will be used to study the effect of antigen crowding on immune response and inflammation. Here, we present the first stages of development of the VM technology. Stable fluorescent liposome formulations were prepared using a highly parallel approach testing combinations of cholesterol and synthetic lipids, aiming to mimic the natural viral envelope lipid composition. The liposomal nanoparticles were analyzed using fluorescence correlation and cross-correlation spectroscopy (FCS, FCCS), UV-VIS and fluorescence spectroscopy, electrophoretic light scattering, and dynamic light scattering. Detergent-solubilized SARS-CoV-2 spike proteins were fluorescently labeled and a detergent-mediated reconstitution method was used to incorporate them into liposomes. Protein insertion was verified using FCCS and FCS to monitor co-localization of labeled proteins and liposomes.

Functional 2D nanostructures via chemical and kinetic control of DNA-oligomer amphiphile self-assembly

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Synthetically accessible two-dimentional (2D) nanomaterials are of great interest due to their prospective applications in electronics, catalysis, and biotechnology. One method of accessing these topologically planar structures is through the supramolecular polymerization of amphiphilic block copolymers (BCPs). The use of DNA-oligomer amphiphiles as the BCPs for construction of supramolecular 2D nanoarchitectures offers the unique opportunity to both introduce functionalized cores in these structures as well as (post)functionalize the surface of the 2D architecture. Such DNA-based 2D nanostructures have not been widely explored, and the few studied thus far have been limited by a lack of control over their shape and size.Here we report the morphological analysis and discuss the hierarchical growth mechanism of 2D nanosheets obtained through the self-assembly of synthetic amphiphilic DNA-oligomers bearing π-conjugated chromophores in aqueous solution. We explore the effect of varying self-assembly methods and polymer lengths on the structural order and size of the nanosheets. The goal is to chemically and kinetically control the formation of the

supramolecular architecture, allowing us to precisely tune the shape and size of the 2D nanosheets. This would enable the creation of synthetically accessible, well-defined, monolayered 2D nanostructures that are viable for practical applications in nanotechnology.

Donor-Chromophore-Acceptor Assembly Visible Light-Driven Oxidation of 1-Phenylpyrrolidine by a Heterogeneous Photoanode

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In recent years, photoredox catalysis and electrochemical synthesis have become an important tool to drive organic transformations. These two technologies are often considered as competing in organic synthesis and hence their merger has been largely overlooked. Dye sensitized photoelectrochemical cells (DS-PECS) can be used to bridge this gap and through tuning the composition, band positions and morphology of the photoelectrode, reactivity and selectivity of the system can be controlled. In this regards, we have developed a Cu(I)-based donor-chromophore-acceptor (D-C-A) triad with specially designed ligands bearing electron donating triphenylamine (tpa) and accepting dipyrido[3,2-*a*:2′,3′-*c*]phenazine (dppz) moieties serving to generate a charge separated state on photoexcitation. The acceptor ligand performs the dual roles of anchoring to the semiconductor surface as well as electron accepting to afford directional charge transport. When grafted onto the zinc oxide (ZnO) nanowires on conducting glass photoelectrochemical studies reveal that this triad, upon photoexcitation can inject electrons directly into the conduction band of ZnO. The resulting oxidizing equivalents are then transferred to 1-phenylpyrrolidine which is subsequently oxidized to generate a radical cation species, that can undergo a coupling reaction to a variety of heteroaromatics.

Post-Synthesis Growth Mechanism of Lanthanide-doped Nanoparticles by Surface Modification

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Understanding the growth mechanisms occurring during the synthesis of nanoparticles has been achieved by varying reaction conditions, such as reaction time, temperature, ligand, and pH. Despite the thorough investigations reported in the literature, the post-synthesis growth mechanism in lanthanide-doped nanoparticles has never been investigated at room temperature. The growth mechanism is reported only for the high-temperature synthesis, by mechanisms such as Ostwald ripening and Oriented attachment. Ostwald ripening involves the dissolution of small nanoparticles in monomers, with successive growth by ripening of the surface of bigger particles with these monomers. Oriented attachment occurs by the alignment of more particles along with a preferential crystal orientation, and attachment of these particles at the interface between particles by the so-called necking.

ABSTRACTS // CHEMISTRY EDUCATION ORAL PRESENTATIONS

Evaluating the impact of English language proficiency on chemistry students' abilities to construct scientific arguments

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In a world grappling with declining trust in science, science education has a responsibility to support students' abilities to make and argue for decisions using scientific evidence and reasoning. As such, chemistry educators have worked to incorporate opportunities for students to construct arguments on assessments (e.g., asking students to justify claims using evidence and reasoning) and researchers have analyzed students' responses to these tasks to learn how to better support students' abilities to construct arguments. However, most investigations have focused solely on students' English language arguments, even though there are upwards of 250,000 international students studying in Canada, the majority of whom come from nations in which English is not a primary language. In this presentation, we will describe our work in developing an instrument to investigate the impact of English language proficiency and history on chemistry students' abilities to construct scientific arguments about a climate change issue: ocean acidification. We will also discuss how aspects of this work can be used to create assessments for courses.

Investigating how the delocalization learning outcomes are being enacted and achieved

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Delocalization (Resonance) is a chemical concept in organic chemistry that influences the chemical reactivity, structure, and physical properties of molecules. Despite the importance of delocalization in chemistry, students' learning in this area has not been studied extensively. The few studies about resonance have identified misconceptions about the subject or propose teaching approaches without evidence to support their effectiveness. Some learning outcomes (LOs) for delocalization have been proposed, but they focus on the initial teaching of the concept. To more comprehensively address resonance concepts in instruction, we identified ten essential learning outcomes about delocalization that a student should be able to demonstrate by the end of an organic chemistry sequence. The goal of our research was to outline how the ten LOs were currently being enacted (*e.g.* taught, practiced, assessed) and achieved (*e.g.* students demonstrating the skill). We investigated how these LOs were taught and practiced by analyzing seven introductory textbooks and how they were assessed by analyzing 51 exams given by seven professors. To determine how the LOs are achieved we analyzed students' final exams answers. In this presentation, the ten essential learning outcomes will be presented along with how they are enacted and achieved.

A pilot study: Investigating how undergraduate chemistry students engage in systems thinking in chemistry education and the impact of collaborative systems thinking tasks

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Chemistry is essential in generating solutions to complex global challenges. However, current approaches to teaching chemistry are often siloed, lacking connections to broader contexts, and can leave students with limited opportunities to consider chemistry's connections to these global issues. Systems thinking (ST) emphasizes dynamic interactions between chemistry concepts and other disciplines and identifies how chemical processes impact or are impacted by societal, economical, and environmental contexts. Therefore, chemistry educators have proposed ST as a way to bridge disciplines and more effectively prepare future scientists and citizens for the interdisciplinary work needed to address these emerging issues. There is currently a need for evidence-based research on this approach. Therefore, a pilot study was designed to identify how chemistry students engage in ST. In the study, we designed a ST task to investigate how collaboration influences the systems being constructed and students' perspectives towards chemistry. With the ability to connect chemistry and the broader learning environment with experience, culture, and knowledge, ST could have a profound

influence on diversity and inclusion in the chemistry classroom. My presentation will highlight the findings of the ST pilot study to date and will share implications for collaborative ST tasks within a remote learning environment.

Electrospray deposition of conjugated polymers in ultra-high vacuum

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Small conjugated molecules (CMs) and polymers (CPs) constitute the class of organic semiconductors and are the basis of a billion-dollar market for organic electronics. Essentially all applications in the field are based on thin films of CMs due to their ease of processability in vacuum via thermal sublimation. However, the equally promising class of CPs are thermally fragile and cannot be evaporated. Therefore, they are exclusively processed via solution-based techniques including spin coating and inkjet printing. There, the presence of the solvent tends to have a decisive effect on the growth behavior of polymer films and significantly limits the control over the film properties. To alleviate this problem, we aim to grow CP films of device relevant thicknesses (10- 100 nm) from the gas phase using electrospray deposition (ESD) in the ultra-high vacuum and control their microstructure in a solvent free environment. This control will provide us information valuable to better understand the complex phenomenology of polymer doping. Our setup allows us to achieve pure films of CPs on atomically clean substates, which will provide further new insight into polymer aggregation without the presence of solvent. In this contribution, I will outline the experimental technique and show some preliminary results.

P3HT:FxTCNQ – dopant strength and concentration are key to charge-transfer complex and ion-pair formation

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The formation of ion pairs (IPAs) and ground-state charge-transfer complexes (CTCs) are the two known mechanisms to occur in the molecular doping of organic semiconductors (OSCs), where the latter CTCs are regarded as detrimental to the doping efficiency. For IPA formation, the p-dopant electron affinity (EA) should be close to or larger than the OSC ionization energy (IE) while, however, frontier molecular orbital overlap can still promote CTC formation instead. Here, we investigate the role of $\Delta E = EA - IE$ for the prototypical system of poly (3-hexylthiophene) (P3HT) p-doped with tetrafluoro-tetracyanoquinodimethane (F4TCNQ) and contrast F4TCNQ with its derivatives of lower degree of fluorination with lower EA. From optical absorption and Fourier-transform infrared spectra we deduce that IPA formation is not only more pronounced for high EA dopants but also at low doping ratios. Further, CTC formation occurs with the highest dopant content even for the dopant of highest EA. Through grazing incidence X-ray diffraction we find that the presence of extended crystallites of a CTC-promoting polymorph is beneficial to conductivity in contrast to CTCs dispersed in pristine P3HT. Our observations illustrate the complex interplay of dopant strength and doping concentration as important factors in the molecular doping of OSCs.

Multivalent Supramolecular Polymers

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Supramolecular polymers are formed by the non-covalent assembly of monomeric units into materials with unique properties and wide-ranging applications. While often made out of single building blocks, many research groups have begun to focus on creating supramolecular polymers which are formed by the co-assembly of multiple compounds. These copolymers are potentially more versatile due to their increased synthetic range. Valency (the number of binding sites on building block A, for building block B to bind or vice versa) is one way these copolymers can be designed to have increased stability. However, increasing valency causes these systems to assemble with unoccupied binding sites leading to imperfections in the copolymer structure. Using thermodynamic analyses we have shown that the copolymerization between polydeoxyadenosine strands of length 15 (polyA) and the small molecule cyanuric acid (CA) initially assembles with an average of only 11 CA molecules, meaning over 25% of binding sites are unoccupied. We show that this is caused by the unusually high valency of the system, and a large entropic driving force which pushes the system to assemble into a distribution of under filled states as opposed to the single most stable state.

Electrospinning of Highly Crystalline Polymers for Strongly Oriented Fibers

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Electrospun nanofibers (NFs) are unidimensional nanostructures formed upon the solidification of a thin electrified jet drawn from a viscous polymer solution. They often demonstrate an exponential increase in mechanical properties at reduced diameters, making them promising candidates for applications in tissue engineering, actuation, and selective filtration. Grasping how polymer chains alter their conformation and orient themselves during the electrospinning process is crucial for understanding the origins of the fibers' resulting properties. Therefore, experimental quantification of molecular orientation is essential for the development of optimized nanomaterials. In this work, polarized confocal Raman spectroscopy reveals that fibers of highly crystalline poly (ethylene oxide) (PEO) maintain a high orientation over a broad range of diameters, in strong contrast with the exponential trend usually reported for amorphous materials. This observation stands for five electrospinning solvents of widely different properties. The results show that the exponential orientation dependence on fiber diameter is not universal and stress the importance of polymer crystallinity on the structure and properties of electrospun nanofibers. This work guides the preparation of fibers with optimal orientation-dependent properties and shows that high crystallinity can afford more robust materials whose performance is less affected by variations in experimental conditions, a valuable feature for most applications.

Analyzing the correlation between the polymer molecular weight and the chain conformation in the vicinity of a polymer/metal interface

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The interfaces between polymers and substrates play an important role in many important processes in polymer science. For example, adhesion, slip under flow, and surface-induced nucleation are all interfacial processes. The chain dynamics and their conformation in the vicinity of an interface are significantly different from the bulk region. Therefore, the development of analytical methods to probe interfacial regions of materials has been the focus of many studies. Sum Frequency Generation Spectroscopy (SFG) stands out as a powerful instrument for achieving this goal, due to its high interface specificity (~1 nm) and suitability for probing buried (hidden) interfaces, a combination of features that are not commonly found in other analytical instruments. SFG is a second-order nonlinear spectroscopy that allows the compositional and semi-quantitative orientational analysis of molecules at interfaces. We have studied the effect of the molecular weight (MW) of polystyrene in the conformation assumed by the polymer in the vicinity of a metal interface using SFG. The results show that in the polystyrene/silver interface, the pendant phenyl ring of polystyrene tends to assume tilt angles larger than 50° with respect to the surface normal and that this angle tends to be larger for lower MW samples.

Influence of phospholipids on the membrane binding of the S100A16 protein in the presence of calcium

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Maintaining the structural and functional integrity of membranes is essential for proper cells function. A recent proteomic study suggests that S100A16 protein participates to the maintain of the membrane integrity in the rod outer segment (ROS) of the photoreceptors in the eye. The protein S100A16, recently discovered, is one of the S100 family proteins for which no protein and membrane interaction has yet been identified. Furthermore, maintain of the membrane integrity is a calcium sensitive process. The polar headgroup composition of the human ROS is 32.5% of phosphatidylcholine, 37.6% of phosphatidylethanolamine and 12.1% of phosphatidylserine. In addition, the polyunsaturated chains constitute between 30-60% of the total lipid fraction in humans. The cholesterol concentration of the discs varies from 5 to 30% between base and summit of ROS. The main objective consists of studying the membrane interactions of the S100A16 protein to better understand its function in maintaining membrane integrity. Specific objectives are: i) to achieve the purification of this protein, ii) to gather information on its membrane interactions, and iii)

to study the influence of calcium on these interactions. Langmuir monolayer model combined with surface tensiometry allows mimicking the composition of cell membranes and performing the membrane binding study.

Uncovering the World of Halogen-Based Architectures in Solid-State Porphyrin Systems using the Cambridge Structural Database

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Porphyrin rings have historically fascinated organic and supramolecular chemists, as well as materials scientists and crystal engineers. We are interested in understanding how the presence of halogen atom functionalities on rigid porphyrin units can lead to the formation of complex solid-state supramolecular architectures, based on halogen bonding and other halogen-mediated interactions. In particular, we recognized the Cambridge Structural Database (CSD) as a rich source of information on halogen-based supramolecular chemistry of porphyrin-based units, accessible through data mining, without the need for extensive synthesis and structural characterization. This presentation will provide an overview of our CSD-based investigation of the supramolecular self-assembly of halogen-substituted porphyrins in the solid state, highlighting the appearance of halogen bonding (X···D, where X = Cl, Br, I and D = N, O, S, Cl, Br, I) and halogen···halogen (X···X) interactions. We will present a synopsis of several non-traditional and underrepresented halogen-mediated interactions in porphyrin systems. The presentation will also provide a systematic analysis of how simpler XB and X×××X interactions cooperatively lead to the formation of more complex motifs in the solid state, that can even be considered examples of halogen-bonded synthons, leading to well-defined classes of 2- and 3-dimensional frameworks

ABSTRACTS // COMPUTATIONAL CHEMISTRY ORAL PRESENTATIONS

Effects of solvated ions on electrochemical CO_2 reduction

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Since the beginning of the 20th century, atmospheric CO_2 levels have steadily risen every year, causing the global temperature to also increase due to the greenhouse gas effect. Chemical conversion is a promising solution to reducing CO_2 levels, as it relies on capturing existing atmospheric CO_2 and converting it into usable chemical feedstocks. One of the major setbacks with this carbon conversion method is the reaction efficiency. This is largely due to H_2 evolution within an electrochemical system competing with the production of CO_2 reduction products. Larger cations can promote the formation of hydrocarbon products over H_2, though this mechanism is not well understood. We present preliminary *ab initio* molecular dynamics (AIMD) simulations of solvated ions in the interfacial regions of Ag, Au and Cu surfaces. Analysis is focused on ion-surface distance, water solvation structure and ion solvation interactions within and across these systems. These findings will allow us to further understand the mechanism of ion effects in electrochemical CO_2 reduction.

Ensemble-based enzyme design can recapitulate the effects of laboratory directed evolution in silico

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The creation of artificial enzymes is a key objective of computational protein design. Although de novo enzymes have been successfully designed, these exhibit low catalytic efficiencies, requiring directed evolution to improve activity. Here, we use room-temperature X-ray crystallography to study changes in the conformational ensemble during evolution of the designed Kemp eliminase HG3 (k_{cat}/K_M 146 $M^{-1}s^{-1}$). We observe that catalytic residues are increasingly rigidified, the active site becomes better pre-organized, and its entrance is widened. Based on these observations, we engineer HG4, an efficient biocatalyst (k_{cat}/K_M 103,000$M^{-1}s^{-1}$) containing key first and second-shell mutations found during evolution. HG4 structures reveal that its active site is pre-organized and rigidified for efficient catalysis. Our results show how directed evolution circumvents challenges inherent to enzyme design by shifting conformational ensembles to favor catalytically-productive sub-states, and suggest improvements to the design methodology that incorporate ensemble modeling of crystallographic data.

ABSTRACTS // BIOCHEMISTRY ORAL PRESENTATIONS

Exposing Small-molecule Nano-entities By a Nuclear Magnetic Resonance Relaxation Assay

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Small-molecules can self-assemble in aqueous solution into a wide range of nano-entity types and sizes (dimers, n-mers, micelles, colloids, etc), each having their own unique properties. This has important consequences in the context of drug discovery including issues related to non-specific binding, off-target effects, and false-positives and -negatives. Here, we demonstrate the use of the T2-CPMG relaxation NMR experiment which is sensitive to molecular tumbling rates and can expose larger aggregate species that have slower rotational correlations. The strategy easily distinguishes lone tumbling molecules versus nano-entities of various sizes. The technique is highly sensitive to chemical exchange between single-molecule and aggregate states, and can therefore be used as a reporter when direct measurement of aggregates is not possible by NMR. Interestingly, we found differences in solution behavior for compounds within structurally related series', demonstrating structure–nano-entity-relationships. This practical experiment is a valuable tool to support drug discovery efforts.

Novel molecular tools to understand the impact of SUMOylation on chosen cellular pathways

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SUMOylation is a post-translational modification that regulates numerous cellular processes including DNA repair. During the SUMOylation reaction, a small protein called SUMO is conjugated to target proteins in order to modify their activity, localization or stability. The ATP-dependent SUMOylation reaction requires the sequential action of an E1 activating enzyme, an E2 conjugating enzyme and E3 ligases. SUMO E3 ligases play an important role in substrate recognition as they promote the formation of protein complexes between SUMO-charged E2 conjugating enzymes and specific substrates. In turn, this facilitates the transfer of SUMO to specific substrates. Malfunctions of SUMOylation reaction has been associated to multiple pathologies such as Alzheimer's disease and cancer. It is however very difficult to understand the impact SUMOylation in those sicknesses, one of the principal reasons being that there is no efficient way to increase SUMOylation of target protein without affecting other pathways. Thus, our goal is to develop molecular tools that will selectively increase SUMOylation reactions of targeted physiological and pathological pathways. Those tools will serve as bases for new therapeutic strategies development.

Screening for reactive metabolites by LC-MS/MS using different trapping agents

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The metabolism of drugs is a process of detoxification, which their solubility to allow their elimination from the body. This process takes place mainly in the liver and can sometimes leads to the formation of reactive metabolites, capable of binding to proteins, and thus inducing cellular toxicity. Therefore, there is a need to study the metabolism of drugs, as well as other xenobiotics, to better understand the potential exposure to reactive metabolites. Various techniques are available to assess the formation of reactive metabolites, the most common is based on *in vitro* trapping by glutathione and the characterization of these adducts by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS). Our goal is to develop an analytical approach to help identify previously uncharacterized reactive metabolites. Ten xenobiotics, with a potential to produce reactive metabolites, have been incubated in the presence of human and rat liver microsomes. Trapping agents with different affinities for reactive metabolites are being evaluated in this study. The use of different trapping agents will allow us to optimize our analysis and provide us with complementary results. Our results have currently highlighted four compounds capable of forming adducts. The characterization of these adducts will be discussed in this presentation.

Characterization of the antibacterial activity of a SiO_2 nanoparticle coating to prevent bacterial contamination in blood products

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Introduction: An innovative strategy to prevent the clinical use of contaminated blood products is to apply an anti-bacterial non-stick coating (MAAC) to the internal surface of storage bags. The objective was to assess the MAAC antibacterial activity (AA) applied on polyvinyl chloride (PVC). **Methods:** The MAAC was deposited on PVC sections (d_{MAAC}=50 µm, A_{PVC}=2500 mm^2) obtained from red cell (RC) and platelet concentrate (PC) bags. The physical properties of PVC ± MAAC were characterized by optical and electron microscopy. AA against two bacteria has been evaluated. The PVC sections were subjected to an inoculum of 5.8 $\log_{10}$CFU/mL (n = 3) for Δt=24h. The bacteria were recovered in neutralizing solution, then enumerated on plate count agar. Cytotoxicity tests were performed with the L929 cell line. **Results:** Electron microscopy revealed a smoother surface for PVC-MAAC. The AA of PVC-MAAC was higher for *S. aureus* with a reduction of 3.8 and 2.2 $\log_{10}$CFU/mL for RBC and PC respectively, compared to a reduction of 3.1 and 1.4 $\log_{10}$CFU/mL for *E. coli*. The cell viability of L929 in the presence of MAAC was greater than 89%. **Conclusions:** This study demonstrates the MAAC AA when applied on the internal surface of blood product storage bags.

Siramesine and lapatinib induce synergetic cell death in advanced prostate cancer cells

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Prostate cancer is the most common cancer affecting men often resulting in aggressive development with poor prognosis. Novel therapeutic strategies include combinational treatments aiming to reduce the negative effects of chemotherapy, such as drug resistance. The use of lysosomotropic agents offers a new possibility since they disrupt lysosomal membranes and can trigger a series of events leading to cell death. In addition, combining lysosome-disrupting agents with targeted inhibitors can induce cell death in different cancer types. Therefore, we hypothesized that lysosomotropic agents alone or in combination with tyrosine kinase inhibitors will induce cell death in prostate cancer cells. We used PC3, DU145 and LnCaP cells and found lysosomotropic agents siramesine and desipramine to induce cell death in a dose-dependent manner. The effects on lysosome membranes and the levels of reactive oxygen species were measured and only siramesine showed a significant increase in lysosome membrane permeability and increased reactive oxygen species. In addition, the combination with lapatinib had a synergistic effect on cell death. These results suggest siramesine alone and in combination with lapatinib are effective in all prostate cancer cell lines. These effects were more prominent in PC3 and therefore hold the potential to treat advanced prostate cancer.

The Importance of the Mitochondrial Unfolded Protein Response in the Fruit Fly (*Drosophila melanogaster*) During Nutritional Stress

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In nature, dietary resources are not always easily available, and this variation has shaped the evolution of cellular processes to ensure suitable mitochondrial, cellular and whole organism functions. The mitochondrial unfolded protein response (UPR^{mt}) is crucial for maintaining mitochondrial functions and for the survival of organisms to this type of stress. In this study, we aimed to evaluate the UPR^{mt} in *Drosophila melanogaster* raised on a series of different diets. We hypothesized that mechanisms involved in the UPR^{mt} are activated after a period of stress and that they alleviate some of the negative impacts from subsequent stressors. Our results on gene expression suggest that the molecular pathways controlling the UPR^{mt} and the ones activated by them are modulated by various diets. Drosophila also show an important increase in mitochondrial respiration when exposed to a high-fat diet, followed by a drastic decreased after few days suggesting mitochondrial dysfunctions. This important reduction is lessened when a fasting period is incorporated before starting the high-fat diet treatment. These results suggest that mitochondrial functions are highly plastic when organisms are confronted with multiple nutritional stress and that the UPR^{mt} is an important process for maintaining adequate cellular functions.

Membrane interaction of retinal proteins S100A1 and S100B

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Müller glial cells, located in the retina, are responsible for the physiological function of the eye nervous system by maintaining tissues homeostasis and cellular maintenance. Within Müller glial cells, membrane-bound guanylate cyclase (ROS-GC1) as well as S100A1 and S100B are colocalized in the membrane of those cells. In Muller glial cells, ROS-GC1 transduces synaptic signal by transforming guanosine triphosphate in cyclic guanosine monophosphate. The activity of ROS-GC1 is actually regulated by S100A1 and S100B in these cells. Thus, alterations in their function could deregulate GC1 synaptic transduction activity leading to ocular pathologies such as diabetic retinopathy or glaucoma where loss of vision is observed. GC1, as well as S100A1 and S100B, are membrane proteins and the regulatory activity of S100A1 and S100B on GC1 is directly influenced by the membrane. Nevertheless, no molecular information on S100A1 and S100B membrane interaction is known. Therefore, the study of membrane binding of S100A1 and S100B is key to understand the regulation of GC1 as well as the retinal synaptic activity. In this study, the Langmuir monolayer model was coupled to surface tensiometry in order to characterize the interactions between phospholipids and our proteins of interest, S100A1 and S100B, in different experimental conditions.

Variability and Diversity in Breadfruit (*Artocarpus altilis* and related hybrids) Starches

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Breadfruit (*Artocarpus altilis* and hybrids of *A. altilis* x *A. marianensis*) is a staple crop of the Pacific Islands that is sustainable, highly nutritious, high in fiber, has a low glycemic index, is devoid of common allergens, and has been granted "Generally Recognised as Safe" status by the FDA. Mature breadfruit contains about 84% carbohydrates, of which about 60% is starch. Previous studies have demonstrated significant variability in the nutritional characteristics of different varieties, but starch has not previously been compared between species and cultivars. We hypothesized that breadfruit varieties, species, and hybrids produce different types of starch. We analyzed starch yield, structure, swelling power, and solubility as well as dietary fiber and starch-bound protein. Across all varieties, breadfruit starches had similar small granule sizes ranging from 3.3 µm to 17.1 µm comparable to rice starch. Starch granules produced by the hybrid varieties were more likely to form aggregates than the granules produced by *A. altilis* varieties. The hybrids also had higher dietary fiber, swelling power, and solubility than the *A. altilis* varieties. These data show that the hybridization of *A. altilis* with *A. mariannensis* impacted starch metabolism and starch characteristics in the fruit.

Use of anion exchange chromatography to study nucleic acid polymorphism under native and denaturing conditions

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The separation and purification of complex oligonucleotide sequences is of importance for the downstream applications of these biological molecules. Methods for purification and characterization of nucleic acids commonly include HPLC, primarily reverse-phase, size-exclusion, and anion-exchange chromatography (AEX). Nucleic acids are diverse molecules which are capable of exhibiting diverse polymorphism. Presence of secondary structure complicates HPLC chromatograms, making interpretation of results and characterization of samples difficult. Previous work has demonstrated the utility of denaturing AEX in simplifying chromatographic profiles of self-complimentary sequences. These methods rely on elution with up to 4 *M* urea at pH 12.4, thereby disrupting secondary structure, allowing meaningful conclusions to be drawn from the simplified chromatograms. Our continuing studies aim to demonstrate the versatility of native AEX in characterization and visualization of polymorphic nucleic acid sequences, namely self-complimentary sequences such as hairpins and G-quadruplex species. Corroborated with RP-HPLC, CD, UV-Vis, and NMR, this work supports the use of AEX for characterization of nucleic acid samples that may be otherwise difficult to interpret due to complex polymorphism.

Photodynamic Inactivation of *E. coli* by a Theragnostic ROS-Activated Dormant Photosensitizer

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Photodynamic therapy (PDT) is an established technique for the treatment of diseases including cancer and bacterial infections. PDT employs photosensitizers which, upon photoexcitation, sensitize singlet oxygen ($^1O_2$), a cytotoxic reactive oxygen species (ROS). With the aim of preventing damage to nearby healthy tissue when light is applied, our group reported a dormant photosensitizer in 2016 that activates upon scavenging ROS to deliver $^1O_2$ specifically in cells under oxidative stress associated with increased ROS generation. The dormant photosensitizer combines a boron-dipyrromethene (BODIPY) photosensitizer with the antioxidant chromanol ring of α-tocopherol as a trap which quenches the excited photosensitizer via intramolecular photoinduced electron transfer (PeT), preventing the sensitization of $^1O_2$. ROS-mediated oxidation of the trap prevents quenching, activating the photosensitizer. We recently developed a second-generation dormant photosensitizer which has dual activity of $^1O_2$ and fluorescence upon activation. Herein I will report on this new compound, and its application in the selective photodynamic inactivation of *E. coli* in which increased ROS levels have been induced by sub-lethal doses of antibiotics.

Identification of small-molecule miR-31 inhibitors through high throughput screening methods

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The number of therapeutically relevant protein targets that are conventionally used for drug discovery is limited. Non-conventional targets, such as microRNA (miRNA), have emerged as promising targets due to their involvement in gene regulation and aberrant expression in many types of cancer. Additionally, literature has demonstrated that the biogenesis of miRNAs can be successfully inhibited by small molecule drugs. In particular, miRNA-31 is overexpressed in metastatic colorectal cancer making it a potential target for the development of improved colorectal cancer treatments. Herein, we report the design and use of *in vitro* high throughput screening assays for the identification of small molecule miRNA-31 inhibitors. Hit compounds will be used for future downstream and structure-activity relationship studies.

Combination BRAF and MEK inhibition is effective in the treatment of *BRAF* non-p.V600 mutant melanomas with co-occurring *NF1* loss-of-function or oncogenic *NRAS* alterations.

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The Mitogen Activated Protein Kinase (MAPK) **RAS-RAF-MEK-ERK** pathway regulates cellular growth and survival. Tumour suppressors like *NF1* negatively regulate this cascade by hydrolyzing active, RAS-GTP to its inactive, RAS-GDP form. Genetic studies have uncovered activating mutations in *BRAF* (p.V600), *N-RAS* (p.G12, G13, Q61) and loss-of-function (LoF) mutations of *NF1* in approximately 50%, 20% and 15% of cutaneous melanoma patients respectively. Past studies have characterized a subset of BRAF non-p.V600 mutants that co-operate with oncogenic NRAS, driving MAPK activation through BRAF mutant-CRAF heterodimers. We observed that *NF1* LoF mutations significantly co-occurred with *BRAF* non-p.V600 mutations in melanoma. However, the mechanism underlying BRAF non-p.V600 mutant co-operation with NF1 loss is unknown. We found that the BRAF p.D594N mutant–identified to co-occur with NF1 loss in melanoma patients–led to MAPK activation upon NF1 knockdown. Interestingly, MAPK activation of this mutant was not due to increased RAF-RAF dimer formation. Thus, we believe that the BRAF p.D594N mutant signals monomerically within an NF1 loss context in contrast to dimerizing within an oncogenic NRAS context. Furthermore, using clinically approved MAPK inhibitors, we found combination BRAF and MEK inhibition effective in the treatment of *BRAF* non-p.V600 mutant melanomas with co-occurring *NF1* LoF or oncogenic *NRAS* mutations.

snr30 in the Assembling Ribosome: Determining the Function of An Essential snoRNA in Ribosome Biogenesis

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The ribosome is essential for the production of proteins in all living cells. The study of ribosome production has implications as a target for rapidly growing cells such as in cancers as well as ribosomopathies. A set of proteins and RNAs known as assembly factors interact transiently with the premature ribosome to facilitate its maturation. One such factor, snR30 is the only essential H/ACA-snoRNA in eukaryotic cells. In order to understand better the role of snR30 within ribosome biogenesis, we created a system for the enrichment of specific stages of the pre-ribosome bound to snR30. Expression of truncations of the pre-rRNA with an affinity tag in combination with the purification of snR30 containing a different affinity tag, will enrich snR30 bound pre-ribosomes from cell lysates. This approach will allow for more precise study of the changes in the structure and composition of the pre-ribosome facilitated by snR30. In this project, we have successfully generated a set of tagged rRNA truncations along with a functional, tagged, snR30 variant and purified both from *S.cerevisiae*. This system will enable us to determine how snR30 facilitates the proper maturation of the eukaryotic ribosome thereby increasing our understanding of the molecular mechanisms during ribosome synthesis.

Phosphorylation-mediated opening of the mid-region of mammalian tropomyosin Tpm1.1 (α)

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The major isoform Tpm 1.1 (α), in the skeletal and cardiac muscles of mammals and birds undergoes a reversible covalent modification by phosphorylation at serine-283. The extent is age-related: fetal heart ~ 0.7 mole per mole vs adult ~ 0.3. To understand the effects of phosphorylation, chromatographically-separated phosphorylated and non-phosphorylated forms of rabbit Tpm1.1(α) were analyzed by limited proteolysis and mass spectrometric peptide mapping, circular dichroism, and F-actin binding. Phosphorylated Tpm1.1(α) is comparatively more susceptible to cleavage by chymotrypsin (at leucine-169) and trypsin (at arginine-133) and heat-induced unfolding in the C-terminal half of the molecule as occurs between 25 and 40 ^{o}C. Phosphorylation also increased the affinity of Tpm1.1(α) for F-actin: Kd, 0.25 μM vs 0.5 μM. The findings reveal: (i) the center of the molecule senses the presence of the phosphate groups more than 100 amino acids away; (ii) phosphorylation opens the central region allowing greater access to the solvent and thin filament protein binding partners such as F-actin and (iii) phosphorylation assists in the formation of thin filaments as would occur early in muscle development.

Shear-induced conformational transition in coiled-coiled protein fibers from freshwater mussels

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The invasive freshwater mussel species *Dreissena polymorpha* (zebra mussels) and *bugensis* (quagga mussels) spread aggressively due in part to their byssus, a collection of protein-based fibres which modulate adhesion underwater. The byssus acts as a tether, and each fibre is stronger, stiffer and better at self-repair than those of the well-characterized marine *Mytilus* mussels. Despite this, little is known about their structure and composition. Here, we used a combination of Raman and FTIR spectroscopy as well as wide angle x-ray diffraction studies to show that native threads contain parallel β-crystallites, analogous to spider silk. Further investigation into the byssus biofabrication process indicate that the byssal precursor proteins are stored as α-helices, and transition to a β-sheet secondary structure during the formation process, similar to structural proteins such as intermediate filaments and keratin. This is a shear induced transformation process and is being attributed to a coiled-coil protein predicted in the mussel transcriptome. Current efforts are aimed at extracting and sequencing this protein to further understand its stress-induced phase transformation.

Connecting Function to Structure of Class II Lanthipeptide Synthetase using Extensive Kinetic Simulations and Tandem Mass Spectroscopy

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Lanthipeptides are a family of unique peptide natural products that contain characteristic thioether rings within their structure. These rings are post-translationally modified into the *C*-terminal core region of ribosomally synthesized precursor peptides (LanAs). In class II lanthipeptides, these modifications are tailored into LanAs through a multistep mechanistic pathway solely catalyzed by a single lanthipeptide synthetase (LanM). These synthetases modify their substrates in an iterative process achieving an extraordinary degree of biosynthetic fidelity. For instance, HalM2 catalyzes the formation of four thioether rings and seven net dehydrations in its precursor peptide (HalA2). Out of 13,440 possible isomers, fully modified HalA2 will consist of only one constitutional isomer. The conformational dynamics of these synthetases most likely play a pivotal role in orchestrating this innate ability. Previously using hydrogen-deuterium exchange mass spectrometry (HDX-MS), we were able to directly observe the conformational dynamics of lanthipeptide synthetases (HalM2) for the first time. Mutations were used to link specific functions to regions highlighted by this technique. We conducted an extensive kinetic study to better clarify the effects on dehydratase and cyclase activity of these variants. In addition, we also conducted an extensive tandem MS experiments on intermediates of these reactions and showed loss of cyclization fidelity.

High Throughput Screening for the Identification of Small Molecule Inhibitors of the pri-miRNA-18a-hnRNP A1 Interaction

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Only 2% of the human genome codes for protein while an overwhelming majority is composed of noncoding RNAs (ncRNAs) whose overexpression has been implicated in diseases such as cancer, neurological disorders, and cardiovascular disease. MicroRNAs (miRs) are short (19-25 nucleotides) ncRNAs that bind at the 3' untranslatable region of target mRNAs, blocking translation and post-transcriptionally repressing protein expression. MiR-18a is overexpressed in many types of cancer, including prostate and lung cancer, causing a reduction in proapoptotic protein expression. Heterogenous nuclear ribonucleoprotein A1 (hnRNP A1) is an RNA-binding protein that has a diverse range of cellular functions, including binding to the primary-miR-18a (pri-miR-18a) transcript to facilitate its biogenesis to functional, mature miR-18a. The knockdown of hnRNP A1 greatly attenuates the expression of mature miR-18a. We hypothesize that the high-throughput screening of a library of pharmacologically active small molecules will yield an inhibitor of the hnRNP A1 – pri-miR-18a interaction, halting the biogenesis of miR-18a. Identified hit compounds will be further evaluated in orthogonal cell-based assays and used in structure activity relationship studies to better probe the roles hnRNP A1 and pri-miR-18a play in various types of cancer and better validate this interaction as potential target for anti-cancer therapeutics.

Exploring the conformational landscape of a lanthipeptide synthetase using native mass spectrometry

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Lanthipeptides belong to the family of natural products called ribosomally synthesized and post translationally modified peptides (RiPPS) which are genetically encoded and modified by specific enzymes to generate biologically active peptides. These systems are attractive targets for rational engineering because the precursor peptides are genetically encoded and the biosynthetic enzymes have relaxed substrate specificity. The enzymes responsible for lanthipeptide biosynthesis (lanthipeptide synthetases) are allosterically activated by precursor peptide binding, and conformational sampling of the enzyme-peptide complex has been suggested to play an important role in guiding the modification process. In this work, we use nanoelectrospray ionization coupled to ion mobility mass spectrometry (nanoESI-IM-MS) to investigate a class II lanthipeptide synthetase (HalM2) and the complex it forms with its precursor peptide HalA2 in their native states, demonstrating that nanoESI-IM-MS is a powerful tool for studying the conformational landscapes and protein-protein interactions of lanthipeptide systems. Through ion mobility studies we show that HalM2 undergoes conformational changes as a result of peptide binding, and also in response to mutations within dynamic elements of the enzyme structure. Altogether, this study reveals the remarkable versatility of the nanoESI-IM-MS approach for probing structure function relationships in RiPP biosynthetic systems.

Dynamics of regulatory and effector CD8 T-cells in mesenteric lymph nodes and blood following very early ARV initiation in acute SIV-infected Rhesus Macaques

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We assessed CD8 T-cell dynamics in mesenteric lymph nodes (MLNs) versus blood in SIV-infected rhesus macaques (RMs) following early antiretroviral therapy (ARV) initiation. 32 female Chinese RMs were enrolled including 25 intravenously SIVmac251-infected animals. Nine monkeys were treated 4 days post-infection with a cocktail of antiretroviral drugs. 5 RMs after ART interruption (8 weeks post-ART initiation) and 4 untreated chronically infected were also studied. Peripheral blood and mechanically isolated cells from MLNs were analyzed by flow cytometry. SIV infection was associated with decreased CD4/CD8 ratio and increased immune-checkpoints expression in both blood and MLNs, which were normalized by early ARV initiation. ARV decreased significantly CD8αα but not CD8αβ T-cells in MLNs. Acute SIV infection resulted in the expansion of CD8 Tregs in blood and MLNs. Early ARV initiation decreased CD8 Tregs only in blood. Additionally, early ARV initiation decreased $CD39^+$ and $CTLA\text{-}4^+$ CD8 Tregs in both blood and MLNs, but still higher levels in MLNs compared

to matched blood samples in the acute phase.Overall, early ARV initiation during acute infection normalized CD8 frequencies and their markers of immune-activation and function in both MLNs and blood, but elevated levels of suppressive CD8 Tregs persists despite early ART in MLNs.

ABSTRACTS // MOLECULAR BIOLOGY ORAL PRESENTATIONS

Revolutionary Phage Therapy

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Bacteriophages, viruses that infect bacteria, occupy a unique position in biology, representing a diverse population with a majority of its genomic function remaining a mystery. By providing an alternative approach to treating bacterial infections, phage therapy provides a cure to chronic life-threatening infections. However, we have barely scratched the surface of bacteriophage therapy, but it promises to be a frontier of bacterial infection control. The aim in my research experience is to gain a better understanding of the diversity of phage that infect *Actinobacteria*. In collaboration with *Howard Hughes Medical Institute* (HHMI) and the University of Pittsburgh, I isolated an *Actinobacteriophage* from a soil sample and proceeded to study its characteristics through plaque morphology and TEM (transmission-electron-microscopy). I discovered a temperate phage displaying a lysogenic life cycle with a siphoviridae capable of infecting *Microbacterium foliorum*. Using GenBank, we sequenced the genomes of several of the bacteriophages we isolated and annotated their respective functions using a suite of bioinformatic tools. Our hope is to gain a better understanding of the function, reproduction and characteristics of bacteriophage, also the diversity and evolution of phages. The ensuing insight will present numerous hypotheses that can be tested through molecular genetic approaches and computationally.

Proximity-dependent labeling with BioID to identify putative interacting partners of HYAL2, a cell surface hyaluronidase

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Hyaluronidases (HYALs) play a significant role in hyaluronic acid (HA) clearance which is essential for normal development. HYAL2 is a surface protein that is speculated to initiate HA degradation because HA accumulates in HYAL2 deficient mice. However, direct assessment of the enzymatic activity of HYAL2 has been challenging. We hypothesized that investigating the proteins proximal to HYAL2 may provide insight into the mechanism of HYAL2 action. We employed proximity-dependent labeling by fusing HYAL2 to BioID2 to enable promiscuous labeling of proximal proteins. After confirming normal expression and subcellular localization of the HYAL2-BioID2 fusion, biotin was added and streptavidin-agarose was used to capture biotinylated proteins. Captured proteins were identified by mass spectrometry and further analyzed by gene ontology and functional annotation. The captured biotinylated proteins after expression of HYAL2-BioID or BioID2 in *Hyal2-/-* mouse embryonic fibroblasts were compared. Of these proteins, 64 were found to be unique to the HYAL2-BioID2 expressing cells. These included enrichments in specific biological processes validated by *t*-test statistics. PPI network of HYAL2 represented 21 proteins as hubs in the network. We have used the BioID system to identify 64 proteins in proximity to HYAL2 that await experimental studies to determine if they are interacting partners.

High-throughput screen of primary human acute myeloid leukemia stem cells identifies novel anti-LSC compounds

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Acute myeloid leukemia (AML) is an aggressive form of blood cancer defined by the uncontrolled proliferation and expansion of immature myeloblasts in the blood and bone marrow, leading to hematopoietic failure. Despite the use of aggressive and cytotoxic standard-of-care drugs, patients often relapse and succumb to the disease partially due to the

chemo-resistant nature of leukemic stem cells (LSCs). Hence, novel therapies targeting the unique biology of LSCs are needed while sparing hematopoietic stem cells (HSCs). We therefore isolated the CD34+ LSC containing fraction of a primary human AML sample (>90% purity) functionally validated to be enriched for LSCs in long-term xenotransplant assays, (Eppert *et al*., 2011), and performed a high throughput screen of 11,166 chemical molecules, counter screened against normal CD34+ cord blood (CB) hematopoietic stem and progenitor cells. From this, 93 highly effective anti-LSC compounds were identified including protein kinase inhibitors, epigenetic modifiers, anti-apoptotic protein inhibitors and glucocorticoids. Glucocorticoids were also previously identified in our small-scale *in silico* anti-LSC screen, where they specifically drive human LSCs to terminally differentiate (Laverdière, I. & Boileau, M., *et al*., 2018). We will now re-validate these hits where the most efficient compounds will be chosen for validation in other primary AMLs.

Dexmedetomidine, a novel anesthetic with neuroprotective effects

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Anesthetics are required for major surgical procedures; however, the precise mechanisms underlying their modes of actions remain poorly defined. Recent animal studies have raised alarms regarding anesthetics' long-term cytotoxic effects, specifically on the nervous tissue. It is thus important to identify potential sites of anesthetic toxicity and then identify mitigating strategies. Here we define the cellular and molecular mechanisms underlying anesthetic-induced toxicity in a cell culture model. We demonstrate the effects of the anesthetic Dexmedetomidine (DEX) (0.05 µM to 10 µM) on rat neuronal viability. We show that DEX does not affect neuronal viability when used below 10 µM. However, in the presence of DEX, neurons exhibited hyperfused mitochondrial network, and more neurite branching - albeit with no differences in synaptic puncta formation. We next asked whether DEX could rescue neurons from neurotoxicity, induced by other anesthetics. Neurons were exposed to sevoflurane, either alone or following pre-treatment with DEX. Pre-treatment with DEX rescued neurons from cell death, and this neuroprotection involved changes to mitochondria homeostasis and morphology. This study underscores the importance of DEX as a conventional anesthetic agent and the one that also plays a neuroprotective role against other agents.

HLA Blockers for potentially treating Rheumatoid arthritis

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Individuals with Autoimmune Diseases such as Rheumatoid Arthritis (RA) experience a slightly increased risk for developing certain types of cancers, including hematological disorders and some solid tumors. RA is an autoimmune disease, caused by improper recognition of self-peptides, particularly human cartilage glycoprotein and type II collagen, by specific human leukocyte antigen (HLA) receptors. Normally T-cell specific for these peptides are destroyed in the thymus before they are released, preventing autoimmunity. However, certain post-translational modifications, especially citrullination, can lead to "self-peptide" recognition by non-self T cells: in the case of RA, one HLA protein, out of about 1700 possible ones, is responsible for 65% of RA cases. If this protein could be blocked, drugs could be developed that interrupt the disease at its root cause without affecting the rest of the immune system; this is the focus of research in the Trant Lab. This presentation will briefly overview the approach, including the drug design, and will focus on the molecular biology work accomplished to date.

Régulation transcriptionnelle de l'expression des cadhérines chez les cellules de sertoli du testicule

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Au niveau du testicule, les cadhérines (Cdh) sont des protéines importantes dans la formation des jonctions adhérentes entre les cellules de Sertoli dans la barrière hémetato-testiculaire. Une expression aberrante de ces protéines causée par des perturbateurs endocriniens peut nuire au développement et à la différenciation normaux des cellules germinales, ce qui peut entraîner une diminution de la fertilité. Par conséquent, une meilleure compréhension de la régulation transcriptionnelle de ces protéines chez les cellules de Sertoli dans le

testicule s'avère nécessaire pour mieux définir leur implication dans la régulation de la spermatogenèse et de la fertilité. Chez les cellules de Sertoli, les gènes codant pour les cadhérines 2 et 3 sont fortement exprimés et corrèlent avec le profil d'expression de facteurs de transcription importants comme les familles AP-1 et SOX. Par les outils bio-informatique, on a trouvé des éléments de régulation pour les facteurs de transcription de ces familles qui sont conservés entre espèces dans les régions promotrices des gènes *Cdh2/3*. L'hypothèse proposée est que les facteurs de transcription Sox et AP-1 coopèrent pour réguler l'expression des cadhérines chez les cellules de Sertoli du testicule.

Two plants, one pathogen, a novel approach gives insight on Prune Dwarf Virus, an understudied virus

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Prune Dwarf Virus (PDV) is an important pathogen of sweet cherry (*Prunus avium L.*) which can cause fruit yield reductions. Host proteins critical for PDV pathogenesis and host responses to infection are not well understood. Label free quantitative (LFQ) proteomics was used to study protein accumulation changes in cherry following PDV infection. A total of 791 proteins were identified from infected and uninfected leaves of orchard grown trees. Many of the proteins with significant accumulation changes ($P < 0.05$) were linked with responses to other pathogens. To better associate cherry proteins with PDV, cucumber (*Cucumis sativus L.*) was infected under laboratory conditions. A total of 1596 proteins were identified, with 87 having significant accumulation changes upon infection. The translationally controlled tumor protein-1 (TCTP1), implicated as a pro-viral protein has not been studied in PDV infection yet showed significant accumulation in the model host. As TCTP1 is important for viral infection in other systems, the cherry ortholog was cloned, and shown to co-localize with the viral coat protein. By using a model host, confounding variables were mitigated. This 'two-plant, one pathogen' approach can lead to identification of important host factors and a better understanding of the plant-pathogen interactome.

ABSTRACTS // ANALYTICAL CHEMISTRY SHOTGUN TALKS

***In vitro* metabolism of Epigallocatechin gallate (EGCG) analogs by LC-HRMS/MS**

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Epigallocatechin-3-gallate (EGCG) and several of its analogs are the major bioactive polyphenols in green tea. Their beneficial health effects include anti-cancer, anti-obesity, anti-diabetes, and neuroprotective effects. Glioblastoma multiform (gliomas) is the most common and deadliest of malignant primary brain tumors in adults. Studies have shown that the use of EGCG may be an effective therapeutic strategy for glioma. The focus of this study was to determine the metabolic pathways involved in the biotransformation of EGCG and seven of its structural analogs, via the formation of reactive oxidative metabolites and methylation. We used liquid chromatography coupled to high-resolution tandem mass spectrometry for the detection of oxidative and methylated metabolites, as well as glutathione conjugates in human and rat liver microsomes in the presence of a NADPH, S-adenosyl methionine and glutathione. High-resolution MS/MS data was used for the investigation of fragmentation pathways and structural elucidation of metabolites. In a follow-up study, EGCG and its analog EGC were incubated with U87 glioblastoma cells to follow its uptake and potential biotransformation in these cells.

ABSTRACTS // ENVIRONMENTAL CHEMISTRY SHOTGUN TALKS

Reconstructing Ancient Maya Population History Using Faecal Stanols

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The analysis of faecal stanols in lake sediment cores offers a novel opportunity to reconstruct human population change, assuming that faecal stanol concentrations accurately relate to relative human populations. The ancient lowland Maya of Central America represents an important ancient society whose demographic dynamics are still being reconstructed. We interpret the faecal stanol record in a sediment core retrieved from a lake adjacent to the archaeological site of Itzan, an ancient population centre in the southwestern Maya lowlands. The sedimentary faecal stanol record from Laguna Itzan implies centennial- and millennial-scale changes in local human populations from 3300 years BP to the present. Variability in faecal stanol concentrations is broadly consistent with archaeological patterns of regional societal change across the Maya lowlands, but also implies an earlier presence of humans at this site than is indicated in Itzan's archaeological record. Our work shows that faecal stanols are potentially strong proxies for human population dynamics and land-use change such as deforestation and agriculture through time.

ABSTRACTS // INORGANIC CHEMISTRY SHOTGUN TALKS

Mixed-linker metal–organic frameworks for the removal of organic pollutants from water

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Metal–organic frameworks (MOFs) are a relatively new class of materials, which have gained significant attention from the scientific community in the past 10-15 years. The interest in MOFs comes from their unique properties, which include tunable structure, large surface area, extensive porosity, and a high degree of crystallinity. Because of these characteristics, MOFs have been used in several areas, such as gas storage, ion-exchange, drug delivery, chemical sensing, catalysis, and adsorption. In this presentation, new mixed-linker MOFs based on the Zr-CAU-28 platform will be discussed. The parent Zr-CAU-28 is comprised of hexanuclear clusters of zirconium bridged by furan-2,5-dicarboxylic acid (FDA) linkers. By incorporating a second linker with less compatible coordination geometry, the adsorption properties of the MOF can be tuned. The adsorption of organic contaminants, reusability, and stability of these MOFs will be presented.

Two for One: Reactivity of Nickel SNS Bis(thiolate) and its Ni(N_2S_2) Isomer

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In contrast to its Ni SN thiolate-imine analog, thermolysis of our Ni SNS bis(thiolate) complex (**1**) does not cleanly afford the Ni(N_2S_2) isomer (**2**). However, electrochemical studies show that reduction of **1** gives $\mathbf{2}^-$ quantitatively. The latter is then readily oxidized using ferrocenium salts to give a high yield of **2**. The CV of isolated **2** also shows a second reversible reduction wave, yielding the diamagnetic zerovalent Ni complex $\mathbf{2}^{2-}$. In this presentation, we compare the reactivity of **1** with that of the three redox states of **2**.

X-Ray Diffraction Structures of Bulky *N,N'*-Disubstituted Aryl Amidines : the *N,N'*-Bis(2,6-diisopropylphenyl)-4-pyridylamidine

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Amidine compounds are well developed in organic chemistry and they are also good chelators for transition metals. The complexes of their sterically demanding derivatives, in particular, found widespread use in catalysis and polymerization reactions. Herein, we report the synthesis and the solid state structure of *N,N'*-bis(2,6-diisopropylphenyl)-4-pyridylamidine(1)which is a symmetrically *N,N'*-disubstituted arylamidine containing a 4-pyridyl substituent on the carbon

atom of the N–C–N linkage and bulky 2,6-diisopropylphenyl groups on the nitrogen atoms. It crystallizes in the *Z-anti* configuration and its amidine C—N bonds present amine [1.368 (1) Å] and imine [1.286 (1) Å] features. Intramolecular hydrogen bonding interactions are present in the structure together with intermolecular N—H···N and C—H···N interactions linking the molecules in chains along the a and caxes.A comparative analysis of 1 within the familiy of other reported bulky *N,N'*-bis(2,6-diisopropylphenyl)arylamidines is also presented.

Design of Base Metal Catalysts for Bifunctional Catalysis Utilizing Biomimetic SNS Ligands

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Transition-metal complexes that utilize metal-ligand-cooperativity (MLC) by inclusion of redox or Lewis acid/base functionality in their ligands have extensive applications in homogeneous catalysis. Bifunctional catalysts based upon earth abundant first-row transition metals are especially sought after for their economy and low toxicity, and have been shown to facilitate catalytic transformations equal or superior to that of the noble metals. While many ligand moieties for bifunctional applications are known, the influence of hard or soft ligand functionalities in catalysts is not at well studied. Both amido and thiolate functionalities are known to act as Lewis bases in the activation of E–H (E = B, Si, N) bonds, however, less is known about the relative efficacy of these moieties in analogous catalytic species. Two new NHC-Cu-[κ^2-SNS] complexes were synthesized to directly compare the bifunctional activity of a hard amido vs a soft thiolate donor in extremely efficient outer-sphere hydroboration and hydrosilylations. Mechanistic studies involving an outer-sphere mechanism have led to the design of associated Mn complexes allowing for the study of a divalent Mn(II) catalytic system.

Electrocatalytic Generation of H2 from Neutral Water in Acetonitrile Using Ni(II)"PN3P" Pincer Supported Complexes with Ligand Assistance

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University of Ottawa

In an attempt to produce Hydrogen-as a promising and environmentally benign energy carrier- from neutral water, we report two air-stable nickel(II) complexes, [Ni(k3-2,6-{Ph2PNMe}2(NC5H3)Br2] , nickel(II) [Ni(k3-2,6-{Ph2PNH}2(NC5H3)Br2] which are capable of efficient electrocatalytic production of H2 from mixed water/acetonitrile solutions at potential of -2.7 V. These catalysts also are capable to reduce stronger proton source such as phenol and acetic acid in lower potentials(-2v). Bulk electrocatalytic studies showed that the catalyst functions with a moderate Faradaic efficiency and turn over frequency. DFT computations support the role of the PN3P ligand as a shuttle to transfer of protons to the metal center.

Functionalization of Semiconductor Surfaces Towards Solar Energy Conversion: Morphological Control, and Photonic Crystals

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Concordia University

Through the tailoring of semiconductor surfaces, a myriad of favourable properties can be obtained and tuned. In the present work, different surface-bound particle morphologies of cuprous oxide (Cu_2O) are obtained via electrochemical deposition using common compounds as additives (e.g. citric acid, sucrose, oxalic acid, etc.). Resulting cubic and octahedral morphologies of Cu_2O present different surfaces with different surface energies and charges, allowing unique interactions with various substrates in photochemical transformations. This is most easily demonstrated via the preferential degradation of cationic versus anionic dyes. By introducing a repeating structure to the semiconductor, a photonic stop band is obtained, resulting in the trapping and guiding of light. By tuning the lattice size of the repeating structure, it is possible to selectively trap light of a target energy, matching that of the absorbance of a photocatalyst. This may result in improved catalytic efficiency and the need for a reduced catalyst loading. Along with accessible synthetic

methods, this leads to the fabrication of inexpensive devices to drive photocatalytic processes, with a large potential for scalability.

ABSTRACTS // NANOCHEMISTRY SHOTGUN TALKS

O^6-Alkylguanine DNA Alkyltransferase Mediated Disassembly of a DNA Tetrahedron

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DNA tetrahedron structures have been explored as drug delivery platforms that release their payload in response to triggers such as light, chemical agents or hybridization of release strands. Tetrahedron DNA structures were formed by the assembly of three-way junction (**TWJ**) oligonucleotides containing *O*^{6}-2'-deoxyguanosine-alkylene-*O*^{6}-2'-deoxyguanosine (butylene and heptylene linked) intrastrand cross-links (IaCLs) lacking a phosphodiester group between the 2'-deoxyribose residues. The DNA tetrahedra containing **TWJs** were shown to undergo an unhooking reaction by the human DNA repair protein *O*^{6}-alkylguanine DNA alkyltransferase (hAGT) resulting in structure disassembly. The unhooking reaction of hAGT towards the DNA tetrahedra was observed to be moderate to virtually complete depending on the protein equivalents. The dismantling of DNA tetrahedron structures by a DNA repair protein contributes to the armamentarium of approaches for drug release employing DNA nanostructures.

A promising new imaging tool for human cells: amine passivated fluorescent carbon dots

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Carbon dots are a nanomaterial with interesting optical properties and have been touted to have the potential for use in studies of cell physiology and medical applications. Although to date they have been reported to have low cytotoxicity, their fluorescence and cellular uptake are not well understood, and can be influenced by their surface composition. Here, we synthesized five different amine passivated carbon dots with different nitrogen content, using a microwave-assisted technique. The physico-optical properties of the dots were characterized using transmission electron microscopy, UV-VIS and Fourier transform infrared spectroscopies. Moreover, we used WST-8 assays to assess their cytotoxicity, and epifluorescence microscopy to determine their uptake in human foreskin fibroblast cells (HFF1). These studies suggest that these carbon dots represent a promising avenue to pursue and have the potential for use as an imaging tool.

ABSTRACTS // CHEMISTRY EDUCATION SHOTGUN TALKS

A multi-institutional, longitudinal study investigating various curricular approaches to teaching and learning organic chemistry

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In 2012, the Department of Chemistry and Biomolecular Sciences at uOttawa reformed the organic chemistry curriculum from a functional group-based approach to patterns of reaction mechanisms approach. Students in a traditional curriculum often resort to rote memorization without understanding the underlying patterns of reactivity. We have started to investigate the effect of this new curriculum and found that students in courses following this curriculum are better at proposing mechanisms for familiar and unfamiliar questions but often see surface features rather than meaningful patterns. An evaluation of this curriculum has been underway at the University of Ottawa and other similar curricula have been proposed. However, no large-scale study of these curricula has ever been carried out to better understand the impacts of various curricular approaches for teaching organic chemistry. The present study investigates four aspects of learning organic chemistry: 1) Students' abilities to organize reactions based on mechanistic patterns 2) Students' knowledge of reactivity principles, 3) Students' abilities to transfer organic chemistry knowledge to other

disciplines, and 4) Students' self-efficacy beliefs towards organic chemistry. During this talk I will present the study's design and preliminary findings.

ABSTRACTS // PHYSICAL CHEMISTRY SHOTGUN TALKS

Investigations on the Aggregation Behavior of an Ionic Liquid in Water + Carbohydrate Solutions – A Review

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In this paper, attempt is made to examine the effect of two structurally different sugars (xylose, glucose) on the micellization behavior of ionic liquid-based surfactants i.e. 1-decyl-3-methylimidazolium bromide ([C_{10}mim][Br]) and 1-decyl-3-methylimidazolium chloride ([C_{10}mim][Cl]) which are different in counter ions, via conductivity measurements at 298.15 K. Through electrical conductivity measurements, the values of the degree of ionization of the counter ions on the micelles (α) and thermodynamic parameters of micellization (ΔG_m) for [C_{10}mim][Br] and [C_{10}mim][Cl] in aqueous carbohydrate solutions were determined.

A review on the aggregation study of an aqueous solution of hydrophilic ionic liquid in the presence of conventional surfactants

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The review summarises the studies carried out to investigate the aggregation behaviour of a tri-substituted imidazolium based hydrophilic ionic liquid, 1-butyl-2,3-dimethyl imidazolium bromide in the presence of external additives, herein conventional surfactants cetyltrimethylammonium bromide(CTAB) and tetradecyltrimethylammonium bromide (TTAB) by employing various techniques such as conductance, fluorescence, ^{1}H NMR spectroscopy and dynamic light scattering (DLS). The aggregation parameters such as CMC, degree of counter-ion dissociation, aggregation number, aggregate size and the various thermodynamic parameters such as ΔG_m °, ΔH_m° and ΔS_m° have been evaluated in order to study the interactions among the ionic liquid and surfactants investigated.

Characterization of Structured Films of Cholesteryl Oleate Using Surface Sensitive Techniques.

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The tear film lipid layer (TFLL) reduces the surface tension of the tear film and assists with its re-spreading upon blinking among many other important roles at the surface of the eyes. Hence, understanding TFLL has been of interest in surface structure-function relationship studies. TFLL consists of a polar lipid monolayer at the aqueous tear film interface topped by a non-polar lipid multilayer separating the tear film from environment. Cholesteryl esters are non-polar lipids comprising 30-45% of TFLL and together with wax esters (30-50%), they create the TFLL non-polar multilayer (up to 93% of its composition). Cholesteryl oleate is a cholesteryl ester used in artificial TFLL models representing its non-polar layer. Despite its use in TFLL models, there has not been a study of cholesteryl oleate's 2-dimensional crystalline structure at air-water interface. In this presentation, results of the study of cholesteryl oleate films on PBS buffered subphase is reported using Langmuir balance surface characterization techniques. The films' morphology is visualized using Brewster angle microscopy. Moreover, using highly sensitive synchrotron-based X-ray surface characterization techniques, including grazing incidence X-ray diffraction (GIXD), X-ray reflectivity (XR) and grazing incidence X-ray off-specular scattering (GIXOS), characteristics of cholesteryl oleate's structured films at air-buffer interface are reported.

Cyclopropene Core-based Molecules as Strong Electron Acceptors in Organic Semiconductors

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The p-doping of organic semiconductors, that is conjugated organic molecules (COMs) and polymers (CPs), is typically done by using strong molecular acceptors as dopants. In principle, high doping efficiency is achieved with dopants of high electron affinity (EA) to promote electron transfer between CP/COM and the dopant molecule. This process leads to an increase in the number of mobile charges (holes) in the semiconductor host, which translates into an increase in conductivity by multiple orders of magnitude. However, p-type molecular doping of COMs/CPs with high IEs beyond 5 eV is still a challenge as it requires p-dopants of an EA in that range. Recently, a new generation of dopants has been presented to improve the doping efficiency which are based on a cyclopropane core, the strongest example being hexacyano-trimethylene-cyclopropane (CN6-CP) with an EA of 5.87 eV and modification of CN6-CP with only three cyano groups (TMCN3-CP) has recently been proposed shows an EA of 5.5 eV. In this project, we want to explore the feasibility of different substitutions at the cyclopropane core such as pentafluorophenyl (PFP) to yield PFPCN3-CP as a first step. We expect the PFP substitutions to increase its doping efficiency.

ABSTRACTS // COMPUTATIONAL CHEMISTRY SHOTGUN TALKS

The Exchange-Correlation Factor Model in Density Functional Theory

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Density Functional Theory (DFT) is the most widely used approach for electronic structure calculations. In the Kohn-Sham scheme, only the exchange-correlation energy E_{xc} needs to be approximated; to this end, we model the spherically averaged exchange-correlation hole $\rho_{xc}(\boldsymbol{r},u)$, which represents the reduction of the electronic density at a distance u from a reference electron at a position $\boldsymbol{r}$. Previously in our group, an exchange factor $f_x(\boldsymbol{r},u)$ was developed to approximate the exchange hole $\rho_x(\boldsymbol{r},u)=f_x(\boldsymbol{r},u)\rho(\boldsymbol{r},u)$. In this expression, $\rho(\boldsymbol{r},u)$ is the angle average of the electron density over all possible orientations of $\boldsymbol{u}$. This method is a variation of the *Weighted Density Approximation* (WDA) and it has the potential of being one-electron, self-interaction error (SIE) free. Furthermore, our group developed a correlation factor ansatz in which the exchange hole yielding the exact exchange-energy per particle multiplies the correlation factor $\rho_{xc}(\boldsymbol{r},u)=f_c(\boldsymbol{r},u)\rho_x(\boldsymbol{r},u)$. Our previous models of f_c were not SIE free, however. To rectify this problem, we are developing an exchange-correlation factor to approximate the hole $\rho_{xc}(\boldsymbol{r},u)=f_{xc}(\boldsymbol{r},u)\rho(\boldsymbol{r},u)$. The exchange-correlation factor is constructed by satisfying physical and mathematical constraints. Preliminary results for atomization energies obtained with simple models of $f_{xc}(\boldsymbol{r},u)$ are encouraging and comparable to popular functionals.

A Molecular Dynamics Investigation into the effect of ATP on Ryanodine Receptor 2

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Ryanodine receptors (RyRs) are intracellular calcium ion channels that play a key role in the function of muscle tissue, by releasing calcium ions from the sarcoplasmic and endoplasmic reticulum into the cytoplasm. This action is important for the excitation-contraction coupling mechanism in cardiac and skeletal muscles. Ryanodine Receptor 2 is specifically associated with cardiac muscle, and mutations in RyR2 are linked to several cardiac disorders. It has previously been shown that the binding of ATP increases the activity of RyR2. While the binding site is known, the mechanism of action is not, though it is speculated that interactions between ATP and charged side chains are important. We have used molecular dynamics simulations to study the interactions between ATP and a reduced model of RyR2 in more detail. Our preliminary results illustrate a potential link between ATP binding and stability of the open state.

Q277 stabilizes the cASIC1 desensitized state through electrostatic interactions and retards recovery

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Acid-sensing ion channels (ASICs) are highly-pH dependent and are involved in many biological processes linked to the central and peripheral nervous systems. The desensitization mechanism of cASIC1 has recently been linked to a specific residue, Q277, in the palm domain. Q277 has been suggested to act as a valve in a steric-driven mechanism, controlling the isomerization of L414 and N415 in the β11-12 linker domain. The Q277G mutant was recently observed to recover from desensitization magnitudes faster than the wild type. Q277 is situated nearby acidic residues in the palm domain and is well-positioned to form electrostatic interactions with the side chain of E80 and the backbone oxygen of L414. For Q277G, both hydrogen bonds and steric effects of Q277 are lost. With molecular dynamics simulations, a Q277N mutation is observed to destabilize the hydrogen bond network in the desensitized state, while steric effects are overall maintained. Experimental data for Q277N confirms a greatly accelerated recovery from desensitization, almost as fast as seen in the Q277G mutant. This suggests that the stabilization of the desensitized state is more dependent on the observed electrostatic interactions than the previously hypothesized steric mechanism.

ABSTRACTS // BIOCHEMISTRY SHOTGUN TALKS

Engineering the NADPH specificity of DepB, a novel aldo-keto reductase involved in the detoxification of the agroeconomic mycotoxin deoxynivalenol (DON).

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DepA, a PQQ-dependent dehydrogenase, and DepB, an NADPH-dependent aldo-keto reductase (AKR) partake in the detoxification of the mycotoxin, deoxynivalenol (DON). The latter aids in the pathogenesis of *Fusarium* infections, reducing the quality and yield of cereal grain crops. DON contaminations cost the cereal grain industry millions of dollars annually, moreover, its inherent toxicity also elicits gastrointestinal disorders in both humans and livestock fed contaminated grain. Current DON management strategies involve physical decontamination or marginally effective chemical treatments; however, a holistic approach incorporating Dep enzymes is a promising strategy. A significant impediment is a requirement for the expensive co-factor, NADPH. Protein engineering approaches can address this issue – by 'switching' DepB's co-factor preference to the cheaper co-factor, NADH. DepB was found to catalyze the transformation of 3-keto DON to 3-epi DON with Km and kcat values of 563.9 µM and 2.49 s^{-1}, respectively, using NADPH as a cofactor. The enzyme's Kd for NADPH was determined to be 44.23 µM using the solved crystal structure of DepB, docking experiments with DepB revealed that Arg-291, Gln-295, and Lys-218 may be important for NADPH specificity. Site-specific mutagenesis was performed to replace these residues to enable the enzyme to utilize NADH.

Fluorescent structure-switching aptamers for real-time monitoring of ROS activity

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Reactive oxygen species (ROS) such as hydrogen peroxide and superoxide are key to several biological pathways but are also a major source of damage within the cell. ROS are produced both endogenously, in the mitochondria, and exogenously, from radiation or certain pharmaceuticals. Tracking of ROS dysregulation, or oxidative stress, is of interest to both research and industry for applications including pharmaceutical testing and biosynthesis. While there are currently several tools for this purpose, the existing methods are invasive or cannot detect changes in real-time. RNA aptamers can be expressed within a living cell, to bind to a target and function as part of a detection or response mechanism. Fluorescent RNA aptamers bind to a GFP-inspired fluorophore and cause a dramatic increase in fluorescence. When fused with a second target-binding aptamer, these constructs function as logic gates: upon target binding, the fluorophore-binding region is stabilized, creating a "turn-on" fluorescent switch. Here we present our work designing fluorescent aptamer switches for monitoring ROS activity, using the Broccoli fluorescent aptamer and a previously selected RNA aptamer for the stable oxidation product 8-oxodG. This includes design of an 8-oxodG minimer and optimization of the fused aptamer with an eye to intracellular applications.

Targeting adipogenesis with green tea derived catechins: An impact on the paracrine regulation of triple-negative breast cancer progression

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BACKGROUND: Obese subjects have an increased risk of developing triple-negative breast cancer (TNBC), associated with the chronic low-grade inflammation state. Epidemiological data indicates that increased consumption of polyphenol-rich fruits and vegetables plays a key role in reducing incidence of some cancers. **OBJECTIVES:** To test whether green tea-derived epigallocatechin-3-gallate (EGCG) could alter adipogenesis processes, and whether pre- and mature adipocytes can regulate TNBC invasive phenotype. **METHODS:** Pre-adipocyte differentiation was performed and conditioned media (CM) from undifferentiated and mature adipocytes harvested. Human TNBC-derived MDA-MB-231 real-time cell migration was performed using the exCELLigence system. Differential gene arrays and RT-qPCR were used to assess gene expression levels. Western blotting was used to assess the protein expression levels. **RESULTS:** EGCG inhibit adipogenesis by reducing expressions of adipogenic markers. Induction of MDA-MB-231 migration was seen in response to CM of mature adipocytes, and correlated with the induction of the STAT-3 signaling pathway. This invasive phenotype was prevented by EGCG, the JAK/STAT inhibitor Tofacitinib, as well as upon STAT-3 gene silencing. **CONCLUSION:** Factors secreted from mature adipocytes play key roles in the paracrine modulation of TNBC cells invasive phenotype. Dietary interventions may prevent the onset of the proinflammatory obesogenic environment that favors cancer development.

Genome mining of Novel Class II Lanthipeptides from Actinomycetes

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Lanthipeptides, a subfamily of ribosomally synthesized and post-translationally modified peptide (RiPP) natural products, are characterized by the presence of thioether rings that are installed through a two-step post-translational modification involving lanthipeptide synthetases. These synthetases are separated into four distinct classes based on how they catalyze the dehydration of serine/threonine residues in the precursor peptide followed by intramolecular addition of cysteine residues onto the dehydration sites to install the thioether rings. Most lanthipeptides are known for their antimicrobial activity through disruption of cell wall biosynthesis, which has garnered the use of some as food preservatives for decades with limited emergence of antibiotic resistance. Others display biological activities such as antiviral, antiallodynic, antifungal, cytotoxic, and morphogenic. To this end, finding structurally novel lanthipeptides has the potential in identifying natural products with interesting functional diversity. Lanthipeptides are attractive for genome mining based approaches due to their small gene clusters, precursor peptides encoded nearby their modifying enzymes and their genetically encoded peptide sequence can be used to predict novelty. In this study, we aimed to use genome mining based tools such as RODEO (Rapid ORF Description & Evaluation Online) followed by cloning and heterologous expression to characterize structurally novel class II lanthipeptides from actinomycetes.

Structural characterization of SUMOylation events in *Arabidopsis thaliana,* a post-translational modification involved in environmental stress response

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As sedentary organisms, plants cannot escape the negative consequences of climate changes which affect their growth and development. It is indeed expected that demographical increase, environmental stresses such as drought, flood, high salinity, and land degradation will put pressure on the agricultural industry in Canada. Recently, studies have shown that SUMOylation, a post-translational protein modification, is involved in environmental stress response. This modification intervenes in the gibberellin signaling pathway. Gibberellins constitute a large family of phytohormones that play different roles in growth, development, seed germination, flowering, and stress response.

The main objective of this study is to identify the molecular determinants involved in the Gibberellin response and the contribution of SUMOylation in the regulation of this pathway in *Arabidopsis thaliana*. To reach this goal, we have

produced, and purified proteins of the gibberellin and SUMOylation pathway in *E. coli*. We will soon analyze the interactions between proteins of this pathway through biophysical measurements and elucidate the tridimensional structure of reconstituted protein complexes. On the long term, this characterization will allow us to isolate and produce plants, capable of resisting stresses.

B-factor analysis suggests that *L*-lysine and *R, R*-bisLysine allosterically inhibit *Cj*.DHDPS Enzyme by decreasing its protein dynamics

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In *Campylobacter jejuni (Cj.)* , dihydrodipicolinate synthase (DHDPS) catalyzes the condensation of pyruvate (pyr) and (S)-aspartate-β-semi-aldehyde (SAS) to form dihydrodipicolinate. *Cj*.DHDPS regulates an essential step in the biosynthesis of *L*-lysine (Lys) and meso-diaminopimelate in bacterial cell wall synthesis. In our study, the normalized B-factors calculated from crystallographic data suggested that Lys and synthetic bisLys inhibitors allosterically inhibit the enzyme by reducing mobility in the regions that undergo transient conformational fluctuations to facilitate the diffusion of substrate Pyr in the active site for catalysis, consistent with published HDX-MS dynamics studies. The normalized B-factors also showed that bisLys allosterically inhibits DHDPS Y110F lysine insensitive mutant by rigidifying these flexible regions. The B-factor analysis suggest that flexibility in the regions (β8, α9, α10, α11, L20, and α12) may be vital for substrate turn over and catalysis. Normalized B-factors of DHDPS and its Y110F mutant with and without inhibitors in different space groups showed similar flexibility patterns, suggesting the reliability of our B-factors analysis**.**

Circular dichroism study of DNA conformations at biologically relevant concentrations

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Circular dichroism of nucleic acids has been typically carried out at sample concentrations around 10 mM, which is far lower than nucleic acid concentrations in biological systems. Attempts to study nucleic acid conformations by CD at higher concentrations using 10 and 1 mm pathlength cuvette led to the artifacts, and the results were impossible to interpret. By shortening the light pathlength of cuvettes to 0.1 and 0.01 mm, we now report the first CD profiles of nucleic acids at mM ranges of concentrations, which are relevant to nucleic acid concentrations in cellular cytoplasm and nucleus. These CD experimental conditions will allow future conformational studies of nucleic acids under biologically relevant conditions.

Drug-derived DNA damage as a predictive biomarker in personalized medicine

L. Wang*, M. McKeague

McGill University

Acute lymphoblastic leukemia (ALL) is the most prevalent cancer in children and adolescents. Current frontline treatment relies on DNA damaging drugs which create both inter- and intra-strand DNA crosslinks, causing cytotoxicity most critically in rapidly dividing cancer cells by inducing double strand breaks (DSBs). Despite certain limitations associated with these drugs, they will likely remain at the forefront because they are relatively cheap and function with efficacies similar to newer targeted therapies. While childhood ALL can have a cure rate of up to 80%, relapse is common and often non-responsive to follow-up treatment, thereby greatly contributing to the rate of mortality. Novel biomarkers such as interstrand crosslinks can help streamline the treatment process by stratifying patients and predicting their response to frontline treatment. Towards this goal, we will leverage established DSB sequencing methods to determine the pattern of N7 guanine adduct formation created by chemotherapeutic treatment. A Jurkat cell line and an ALL-SIL cell line were established as model systems and their respective susceptibility and resistance to treatment with cyclophosphamide was established using a cell proliferation assay. These findings lay the groundwork for further development of a biomarker-based tool to predict the best course of treatment for individual ALL patients.

Novel neurodevelopmental genes in *C. elegans*

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Ongoing research with the powerful model *C. elegans* continues to uncover fundamental principles about the mechanisms that drive the development and function of the nervous system. Our goal here is to uncover cellular and molecular mechanisms that mediate neuronal development, including that of dendritic spines. For this, we are studying several genes *mau* (maternal-effect uncoordinated), which are defined by mutations isolated in a screen for maternal-effect viable mutations. *mau* mutant animals display morphological and behavioural defects that vary in penetrance and expressivity. Our phenotypic analyses of *mau* mutants reveal that their locomotion is variably abnormal, with episodes of paralysis, spasms and altered body postures. *mau* mutants have defective axon guidance, including for left/right guidance choice at the ventral midline. Moreover, *mau* mutants display defects in dendritic spines number and distribution, and their synaptic transmission appears affected as well. We are progressing toward molecularly identifying and characterizing the *mau* genes, which will provide insights on how these novel genes contribute to neuronal development, including of dendritic spines *in vivo*.

Defining the bio-nano interactions of lanthanide-doped upconversion nanoparticles

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Background. Lanthanide-doped upconversion nanoparticles (Ln-UCNPs) are at the forefront of nanotechnology. Their unique physicochemical properties are particularly suitable for health-related applications, such as bio-sensors or vehicles for drug delivery. Despite the promise of Ln-UCNPs for nanomedicine, progress is currently limited as their bio-nano interactions are poorly defined. **Methods.** First, we evaluated the toxicity of Ln-UCNPs *in vitro*; cancer and non-malignant cells were used as models. Second, several biomarkers of nuclear organization and function were assessed. This included nuclear lamins, nucleolar proteins, and nuclear transport factors. In addition, Nrf2 and NF-κB were also monitored. These transcription factors provide readout for cellular stress responses. Third, the *in vivo* toxicity of Ln-UCNPs was examined in the nematode *C. elegans*. **Results.** The Ln-UCNPs produced by us did not impair the viability of cultured cells, nucleolar organization, or subcellular distribution of nuclear transport factors. Nevertheless, Ln-UCNPs induced minor morphological changes of cell nuclei and slightly reduced Nrf2 and NF-κB levels in non-malignant cells. *In vivo,* Ln-UCNPs did not accumulate in *C. elegans* and had no toxic effects. **Conclusions.** We have produced Ln-UCNPs; they were evaluated in different model systems. Our results demonstrate that these Ln-UCNPs are suitable for the future development of new theranostic tools.

Elucidating the gene regulatory network underlying gliogenesis in the enteric nervous system

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The enteric nervous system (ENS) is the largest division of the peripheral nervous system. It is organized into two interconnected ganglionated plexuses that control essential functions of the digestive tract. These plexuses are composed of neurons and enteric glial cells (EGCs), which are both derived from neural crest cells. Based on their morphology and topology, four distinct sub-types of EGCs have been identified, all expressing the molecular marker Plp1. However, the regulators involved in EGC diversification remain unidentified. We hypothesize that each EGC sub-type expresses distinct set of molecular markers involved in their diversification. Our first objective is to identify these specific markers via single-cell RNA sequencing of Plp1+ EGCs at different developmental stages. To specifically isolate Plp1+ EGCs, we use genetically modified mouse lines allowing Cre/LoxP-based labeling of EGCs with YFP fluorescence in a tamoxifen-inducible manner (Plp1-CreERT;Rosa26-FloxedStop-YFP). This study has just begun and ongoing work is focused on validating our genetic toolkit for fluorescent labeling the different sub-types of EGCs at chosen development stages.

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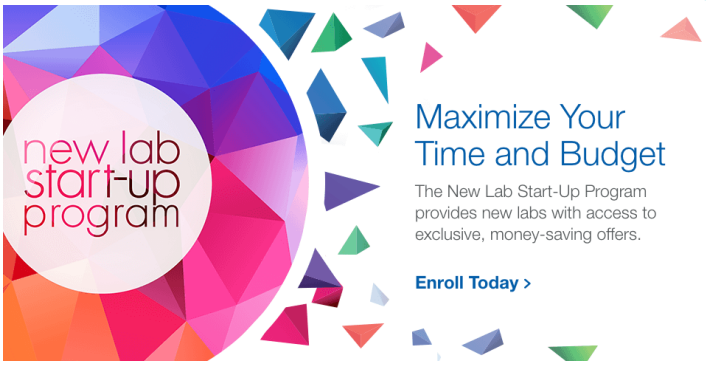
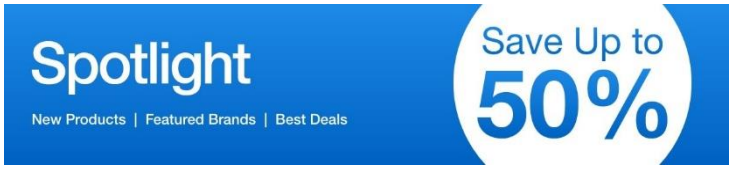
2 Want to win a "Back to the Lab T-shirt" ?

Simple, connect with Sarah in the Fisher Scientific Zoom Room on Nov 20th and let us know about your lab current research. Automatically get a chance to win Back to the Lab Theme T-Shirts

3 Did you move to the new HUB at Concordia?

You are admissible for the New Lab Start Up Promos! Contact Sarah.





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ACKNOWLEDGEMENTS // REMERCIEMENTS

We would like to sincerely thank the participants, judges and sponsors for making this year's CBGRC a success. We extend our gratitude to our guest speakers Dr. Anna Vedda (University of Milano-Bicocca) and Dr. Alexander J. Stirk (Apotex Pharmachem Inc.). Our sincerest gratitude goes to Dr. Christine DeWolf, Hilary Scuffell, Dr. Yves Gélinas, and the Department of Chemistry and Biochemistry for their support and expertise. We would like to thank all our volunteers and the CBGRC organizing committee for all their hard work. We hope you had a wonderful experience at the 23rd CBGRC and we look forward to seeing you all again next year!

The CBGRC Organizing Committee

Nous voulons sincèrement remercier les participants, les juges et les commanditaires pour avoir participés au succès de cette conférence. Nous exprimons notre gratitude à nos conférenciers invités, Dre. Anna Vedda (Université de Milano-Bicocca) et Dr. Alexander J. Stirk (Apotex Pharmachem Inc.). Nos plus sincères remerciements à Dre. Christine DeWolf, Hilary Scuffell, Dr. Yves Gélinas, et le Département de Chimie et Biochimie pour leur soutien et expertise. Nous tenons aussi à remercier particulièrement nos bénévoles et les membres de notre comité d'organisation pour leur dévouement et leurs longues heures de travail. Nous espérons que la 23e CRCSCB fut une expérience très agréable et nous souhaitons avoir le plaisir de vous revoir l'année prochaine!

Le Comité Organisateur de la CRCSCB

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