CBGRC
Chemistry and Biochemistry
Graduate Research Conference

UNIVERSITÉ
Concordia
UNIVERSITY

Welcome to

The Chemistry and Biochemistry Graduate Research Conference

Friday, November 11, 2022

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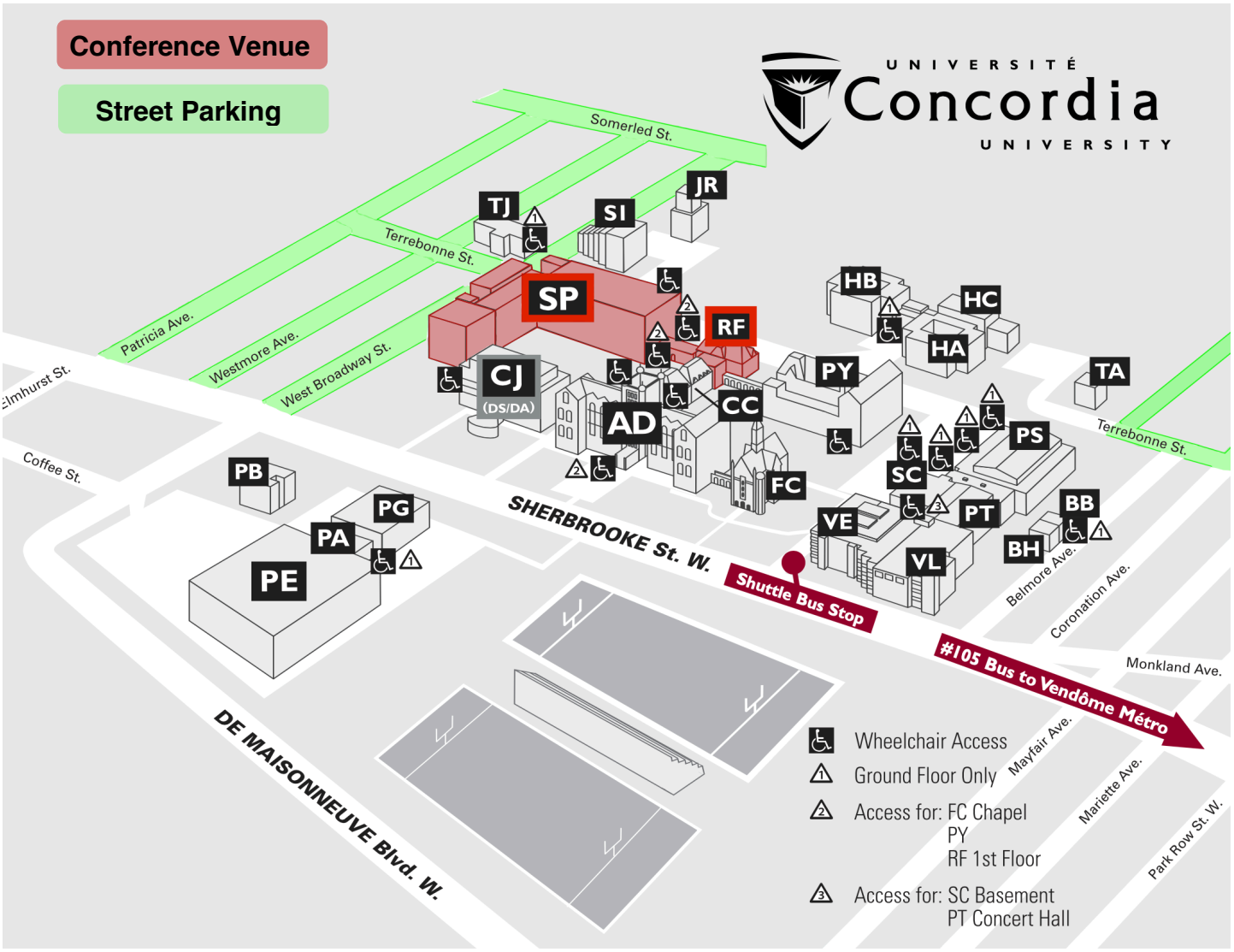
Campus Maps


Conference Venue
Street Parking
UNIVERSITÉ Concordia UNIVERSITY
Somerled St.
Terrebonne St.
Patricia Ave.
Westmore Ave.
West Broadway St.
Elmhurst St.
Coffee St.
TJ
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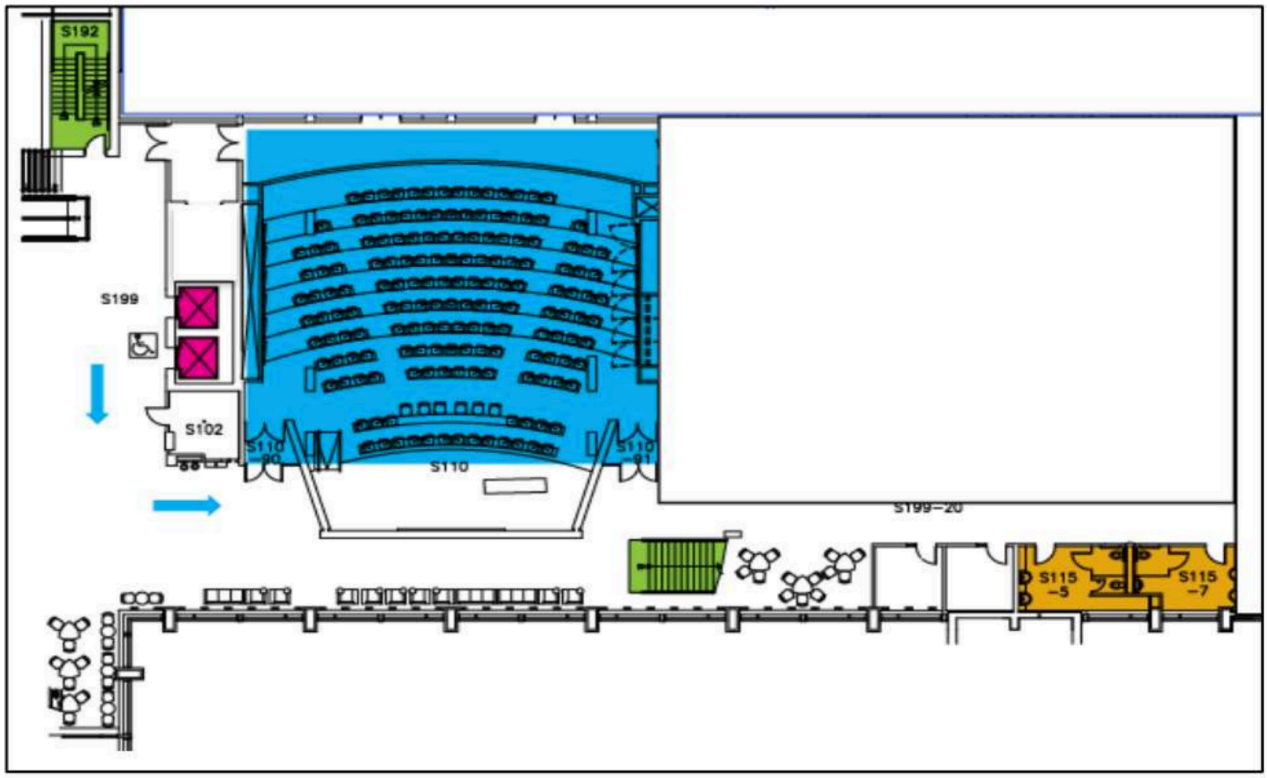
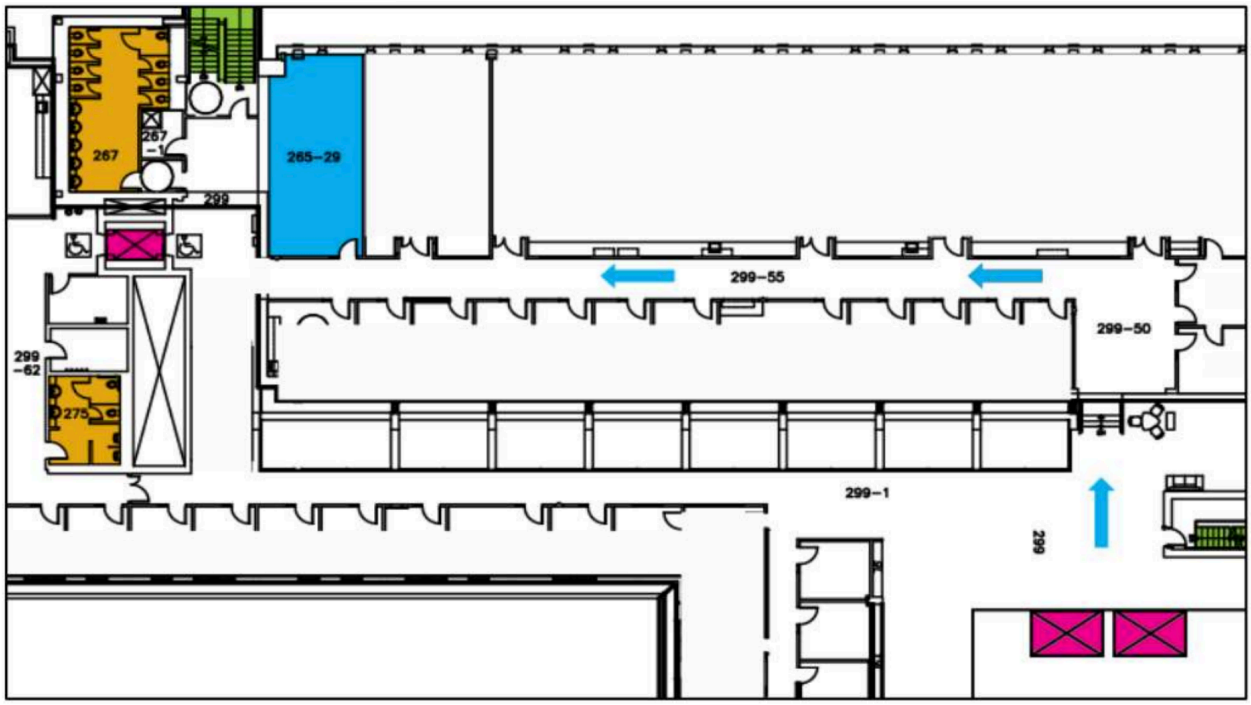
Mariette Ave.
Park Row St. W.
Wheelchair Access
Ground Floor Only
Access for: FC Chapel
PY
RF 1st Floor
Access for: SC Basement
PT Concert Hall

SP – S100

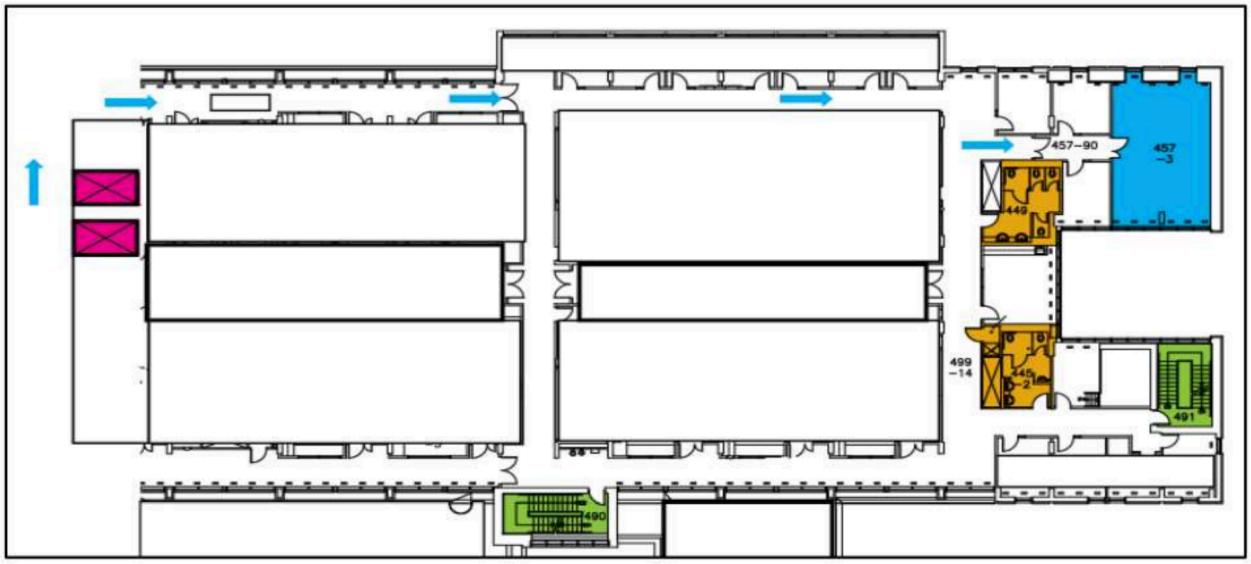


Elevators Stairs Washrooms

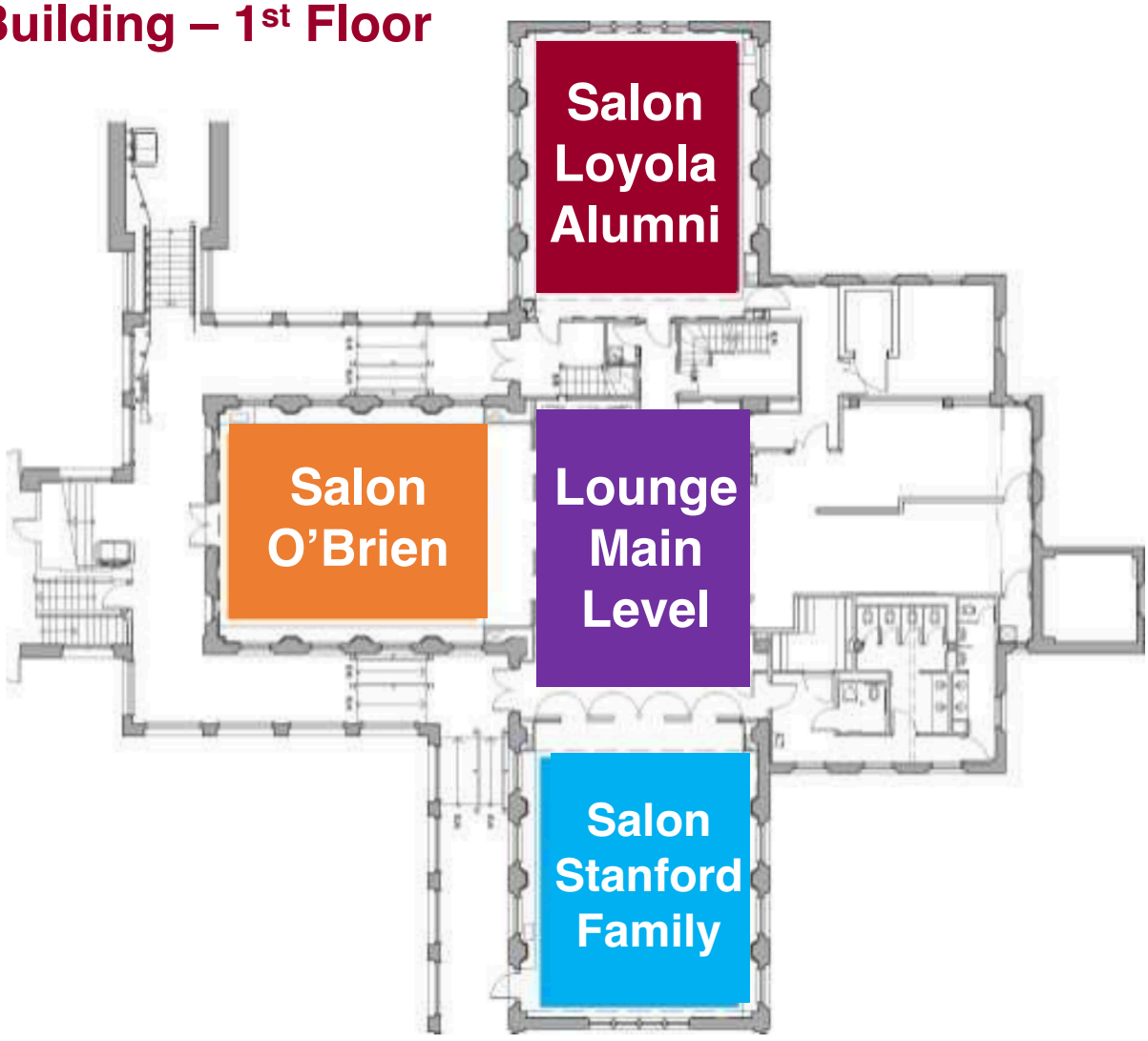
SP – 265.29



SP – 475.03

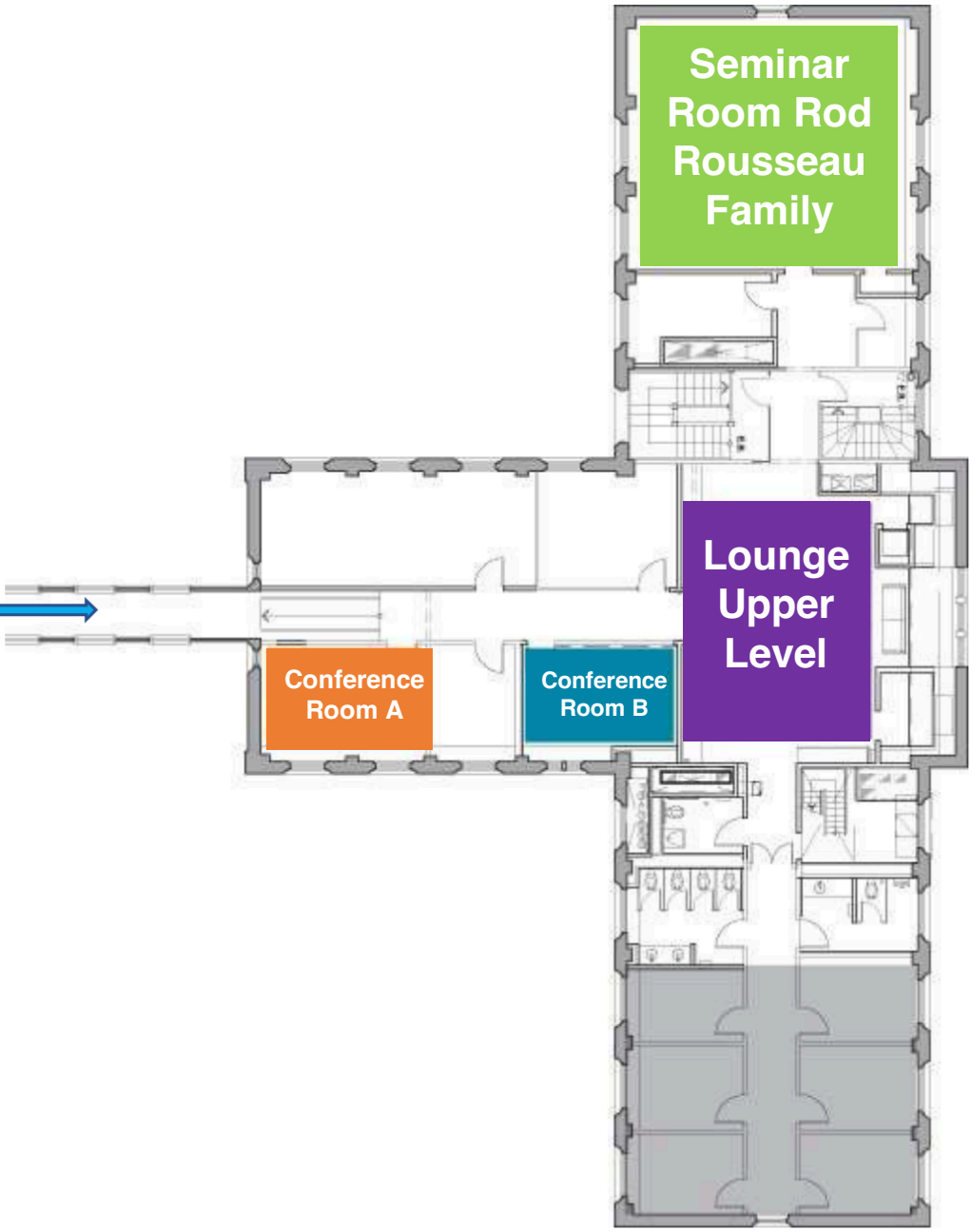


RF Building – 1st Floor



RF Building – 3rd Floor

Enter through CC stairs to 3rd floor



Welcome Note

Dear friends and colleagues,

We are very excited to welcome everyone to the 25th annual Chemistry and Biochemistry Graduate Research Conference. The goal of the CBGRC has always been to gather graduate students, professors, and industry representatives in order to have them share their knowledge and research in a welcoming environment. This year is a special anniversary for the conference, 25 years, and we wish to celebrate the alumni organizers before us who have helped forge a path that has allowed for the conference to flourish into the large event it has become. We are proud to be welcoming over 325 participants, judges, alumni, sponsors and volunteers to be among us for this year's event, and to be joined once again in person by so many of you but also to welcome virtual participants in this hybrid conference. The conference has learned to adapt over the past several years due to the pandemic and we are committed to continue to work all to make this conference an accessible event for all graduate students we hope that this year is an example of that commitment. 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 and hopefully see you all again next year.

The CBGRC Organizing Committee

Chers amis et collègues,

Nous sommes très heureux d'accueillir tout le monde à la 25e conférence annuelle de recherche des diplômés en chimie et biochimie. L'objectif du CRCSCB a toujours été de rassembler des étudiants diplômés, des professeurs et des représentants de l'industrie afin qu'ils partagent leurs connaissances et leurs recherches dans un environnement accueillant. Cette année est un anniversaire spécial pour la conférence, 25 ans, et nous souhaitons célébrer les anciens organisateurs avant nous qui ont aidé à forger le chemin qui a permis à la conférence de s'épanouir dans le grand événement qu'elle est devenue. Nous sommes fiers d'accueillir plus de 325 participants, juges, anciens organizateurs, sponsors et bénévoles parmi nous pour l'événement de cette année, et d'être à nouveau rejoints en personne par un si grand nombre d'entre vous, mais aussi d'accueillir des participants virtuels à cette conférence hybride. La conférence a appris à s'adapter au cours des dernières années en raison de la pandémie et nous nous engageons à continuer à travailler ensemble pour faire de cette conférence un événement accessible à tous les étudiants diplômés. Nous espérons que cette année sera un exemple de cet engagement. Nous tenons à remercier tout le monde pour votre aide à faire du CRCSCB un succès continu, et nous avons hâte d'écouter vos présentations et espérons vous revoir l'année prochaine.

Le comité organisateur du CRCSCB

Guest Speakers

Keynote Speaker – Angelo Filsoa, Ph.D. // 14:30 EST

Biography

Angelo Filosa is the President of PerkinElmer Health Sciences Canada and the Global Portfolio Director for OneSource Professional and Technology Services, where he consults for a variety of organizations – helping to improve lab efficiencies and develop strategic roadmaps for operational improvement initiatives. Prior to PerkinElmer, he was an Associate Director in Chemistry at Boehringer Ingelheim leading analytical chemistry and compound management groups. He also worked in drug development with Eli Lilly and in drug discovery at AstraZeneca. He holds a PhD in Chemistry from Concordia University and is black belt certified in Lean Six Sigma.

Abstract: I Graduated… What's Next?

During this presentation, you'll hear about the different opportunities available for science students to transition into industry with an emphasis on the life sciences. A description of the traditional paths charted by students in research environments, to a look at alternative careers in science that exist outside of the traditional path. Discover the importance of matching skills with jobs and market needs by building your brand and have a chance to ask questions to discover potential new directions for your career.

Alumni Networking Panel // 10:45 EST

Dr. Brigitte Desharnais

Scientific coordinator in toxicology – Development and quality assurance
Laboratoire de sciences judiciaires et de médecine légale (Québec Forensic Science Laboratory)
As a scientific coordinator, I manage the Department of Toxicology's R&D projects and quality assurance activities. I also perform some research work, including statistical analysis, experimental design, and redaction of peer-reviewed publications.

LINKEDIN

Dr. Donald Paquette

Associate Vice President - Analytical R&D
Medicago
Accountable for the design and development of analytical control and characterization programs for vaccine candidates in early to late stage clinical trials.

LINKEDIN

Prof. Fiorenzo Vetrone

Professor
INRS, Université du Québec
A pioneer in the field of rare earth doped upconverting nanoparticles his research interests focus on luminescent nanoparticles and their implementation in multifunctional nanoplatforms for application in biological systems and nanomedicine.

WEBSITE

Mr. Mina Ibrahim

Senior Sales/Operations Manager

ACP Chemicals Inc.

I oversee the customer care, inside sales and supply chain functions for ACP Chemicals. The focus of my work is the overall improvement of the customer experience while improving the company's bottom line via productive and efficiency gains through effective sourcing and production planning.

LINKEDIN

Prof. Rafik Naccache

Associate Professor & Research Chair in Sustainable Multifunctional Nanomaterials (Tier II)

Concordia University

Our research program is concerned with the sustainable synthesis of fluorescent carbon dots and achieving a fundamental understanding of their physico-chemical and optical properties. We then leverage the knowledge gained to engineer nanomaterials and nanoconstructs that can be integrated in sensing, imaging and catalysis applications.

WEBSITE

Dr. Sean Hughes

Science Program Coordinator / Chemistry Teacher

John Abbott College

I have been teaching chemistry for 16 years at John Abbott College. From 2010-2020, I was coordinator of the Pathways Program and in 2021 I became Science Program Coordinator. I have also been involved in educational research in collaboration with SALTISE.

LINKEDIN

Dr. John Manioudakis

Senior R&D Scientist

Intersand Canada

John Manioudakis holds a PhD in biochemistry and a postdoc in nanomaterials from Concordia University. He has mainly worked in analytical and bioanalytical chemistries associated with the pharmaceutical domain. He is currently the Lead Researcher for sister companies Intersand and Blücare Laboratories, where he leads a team of researchers developing animal hygiene products and veterinary devices for the early detection of diseases in animal urine.

LINKEDIN

Dr. Kathryn Balind

Officer of research and development

Groupe de recherche et d'intervention psychosociale (GRIP)

GRIP is an organization that stives to increase awareness related to drug use, and promotes harm reduction practises. In our new drug checking service we use colorimetric reagents, immunoassay test strips, and FT-IR to identify the components in a drug, for the purpose of helping people make informed decisions for their drug consumption. My role involves developing protocols, researching new technologies, writing reports, vulgarizing data and information, and training people who do not have a background in science.

LINKEDIN

Schedule Overview

TIME (EST)	EVENT
7:30	Registration Begins
8:00 – 8:30	Breakfast & Sponsors Exhibition
8:30 – 10:00	Talk Session A
10:00 – 11:45	Poster Session 1*
10:45 – 12:00	Alumni Meet & Greet Networking Session + Coffee*
12:00 – 12:45	Lunch & Sponsors Exhibition
12:45 – 14:15	Talk Session B
14:15 – 14:30	Coffee Break & Sponsors Exhibition
14:30 – 15:30	Keynote Lecture
15:30 – 15:45	Coffee Break & Sponsors Exhibition
15:45 – 17:45	Talk Session C
18:00 – 19:45	Poster Session 2*
18:00 – 22:00	Wine & Cheese*
20:30	Award Announcements

*These events are happening on the 1st floor of the RF building in tandem; presenters will be able to participate in both at the same location

https://concordia-ca.zoom.us/my/cbgrc

Schedule

Talk Session A // 8:30 – 9:45 (EST)

Analytical & Environmental — SP 265.29

8:30 D. Boivin *(Concordia University):* Heart Cutting from a Capillary Array

8:45 M. Lépine *(Université du Québec à Montréal):* Discovering protein biomarkers for ocular mucous membrane pemphigoid in human tears

9:00 R. Maulana *(Concordia University):* Evaluation of Ionic Liquids using Dispersive Liquid-Liquid Microextraction for Metabolomics

9:15 K. Krause *(University of British Columbia):* Rational design of quantum dot surface chemistry for protease detection

9:30 M. Mireault *(Université du Québec à Montréal)*: Semi-targeted LC-HRMS/MS analysis to decipher the effects of acetaminophen on human bile acid profiles.

Organic Chemistry — SP 457.03

8:30 P. Beauclair *(Université de Montréal):* Synthesis of urea-based transporters and their anion transport activity

8:45 X. Bertrand *(Université Laval):* Synthesis of Tertiary Alkyl Fluorides by Hydrofluorination of Alkenes and Deoxyfluorination of Alcohols

9:00 O. Bleton *(Université de Montréal):* A Continuous Flow Platform for Photochemical Macrocyclization of Peptides.

9:15 D. Campbell *(McGill University):* An Organocatalytic oxy-Cope/Michael Cascade Reaction

9:30 C. Cruché *(Université de Montréal):* Investigating a Macrocyclic Strained 1,3-Diyne in "Click" Cycloadditions.

Biochemistry RF 335

8:30 J. Besna *(Université de Montréal):* Screening Indigo Formation for Predicting Substrate Promiscuity in Cytochrome P450 BM3 Libraries

8:45 J. Arciszewski *(McGill University):* Development and optimization of mechanoenzymatic plastic depolymerization: a novel approach to plastic recycling

9:00 N. Reid *(Concordia University):* Schizosaccharomyces pombe tRNA nucleotidyltransferases: A tale of two genes

9:15 A. Fendri *(Université de Montréal):* Cofactor-Free Continuous Flow Biocatalysis System for Potential Low-Cost Applications Using the Cytochrome P450 Enzyme

9:30 C. Gu *(University of Ottawa):* Non-SELEX method for Aptamers Selection to H3 domain peptide of SARS-COV-2 Envelope protein

Physical Chemistry RF 324

8:45 Z. Alinia *(Concordia University):* Phosphole-lipid films: 2D self-assembly, head group interactions, and external effects

9:00 J. Ramos Sanchez *(McGill University):* Superior Photoprotection of Cyanine Dyes with Thio-imidazole Amino Acids to Maximize Photon Budget in Single Molecule Fluorescence Studies

9:15 E. Hamzehpoor *(McGill University):* Synthesis of Boroxine and Dioxaborole Covalent Organic Frameworks via Transesterification and Metathesis of Pinacol Boronates

9:30 S. Charoughchi *(Concordia University):* A novel bulky P-dopant for organic semiconductors

Inorganic Chemistry RF 320

8:45 E. Anderson *(McGill University):* High-throughput studies of Li-La-Zr-O garnet solid electrolytes

9:00 S. Prelaz *(Concordia University):* Thiolated Metal–Organic Frameworks for Ophthalmic Drug Delivery

9:15 J. Ricardo-Noordberg *(Concordia University):* Microstructured Semiconductor Surfaces Towards Enhanced Light Harvesting for Dye-Sensitized Photocatalytic Systems

9:30 V. Lapointe *(Concordia University):* Hybrid Inorganic Perovskite-Photonic Crystal Beads with High Quantum Yields of Photoluminescence

Talk Session B // 12:45 – 14:30 (EST)

Analytical & Environmental SP 265.29

12:45 O. Kuteyi *(Concordia University):* Stability of oxylipins stored on biocompatible solid-phase microextraction (SPME) devices.

13:00 A. Malkawi *(Université du Québec à Montréal)* : A diagnostic electrochemical aptasensor development for sCD80 protein detection in human serum

13:15 E. Mariani *(Concordia University):* LC-HRMS characterization of sulphate and glutathione mycotoxins of 17 mycotoxins found in the Canadian food supply.

13:30 N. Ghafari *(Université du Québec à Montréal)* : Metabolome coverage from targeted and untargeted method

13:45 L. Cougnaud *(Concordia University):* Longitudinal LC-HRMS oxylipin profiling to investigate the atherogenicity of low carbohydrate - high protein diets

14:00 A. Sakaya *(McGill University):* Singlet Oxygen Flux and Membrane Expansion Dynamics Visualized on Giant Unilamellar Vesicles

14:15 K. Sheedy *(Carleton University):* Chemical Derivatization of Glufosinate via Trimethylation Enhancement Using Diazomethane (TrEnDi) for Enhanced Mass Spectrometry Analysis in Canola Samples

Organic Chemistry SP 457.03

12:45 M. Darnowski *(University of Ottawa):* Synthesis of a constitutional isomer of armeniaspirol A, pseudoarmeniaspirol A, via Lewis acid-mediated rearrangement

13:00 A. Fnaiche *(Université du Québec à Montréal):* Development of Small-Molecules TEAD Inhibitors Derived from Flufenamic Acid

13:15 R. Gauthier *(Université Laval):* Gold-catalyzed hydrofluorination of alkynes using hydrofluoric acid

13:30 J. Guerrero-Morales *(Université de Montréal):* Macrocyclization via dynamic kinetic resolution using a chemoenzymatic approach

13:45 R. Hernandez *(Concordia University):* Revisiting the Regioselectivity of Disubstituted Isoxazoles: Ru(II) Mechanocatalyzed Synthesis of 3,4-Isoxazoles

14:00 K. Mckibbon *(Concordia University):* Development of the thieno[3,2-c]isoquinoline scaffold as a potential anti-cancer agent

14:15 E. Ospanow *(Dalhousie University):* Synthesis of exoglycals and exoglycal derivatives as enzyme inhibitors

Biochemistry RF 335

12:45 Y. Habibi *(McGill University):* Exploring the effects of substrate post-translational modification on the structural dynamics of a lanthipeptide synthetase

13:00 S. Heans *(McGill University):* Pantothenamide-Mimicking Compounds: A New Class of Antimicrobial Agents

13:15 C. Hennecker *(McGill University):* Structural polymorphism of guanine quadruplex-containing regions in human promoters

13:30 Y. Kim *(University of Toronto):* A Scalable Hemoglobin Bis-Tetramer Synthesis for Use Towards Pre-Clinical Studies

13:45 A. Kirby *(University of Ottawa):* Mapping Concussion for Early Diagnosis by Molecular MRI

14:00 N.Moghadam *(Université du Québec à Montréal):* Identification of new nucleolar HBZ-associated proteins in chronically HTLV-1-infected cells

14:15 J. Pierscianowski *(McGill University):* The bacterial itaconate degradation pathway: an immune system evasion mechanism and antimicrobial target

Molecular Biology RF 324

12:45 P. Singh *(Concordia University):* Evolution of Plasmid-encoded *CTX-M-15* Gene Against a Set of Beta-lactam Antibiotics

13:00 A. Bouchard *(Université du Québec à Montréal):* Novel molecular tools to increase SUMOylation of target protein

13:15 F. R. Chowdhury *(Concordia University):* Exploiting evolution: Chloramphenicol resistance impairs evolution of resistance to antibiotics

13:30 M. Côté-Cyr *(Université du Québec à Montréal):* Genetic engineering of *Bacillus subtilis* for usage in living functional materials

13:45 M. Jeffs *(Queens University):* Development of a Whole-Cell Biosensor for β-Lactamase Inhibitor Discovery

14:00 M. Mora Ochomogo *(Queens University):* Sheltering of B-lactam-susceptible bacterial strains by B-lactamase-producing bacteria

14:15 H. Almousa *(Concordia University):* Biallelic variants in *TRAPPC6B* cause neurodevelopmental disorder in humans and suggest a defect in TRAPP II-specific function

Inorganic Chemistry RF 320

12:45 A. Grover *(University of Vermont):* Characterization of a Ferryl=oxoheme form of *Staphylococcus aureus* IsdG

13:00 A. Hebert *(McGill University):* Combinatorial Study of Systematic Aluminum Substitution into NMC Cathode Materials

13:15 V. Quezada Novoa *(Concordia University):* Rare-earth metal–organic frameworks with a pyrene-based linker for the photo-oxidation of a sulfur mustard simulant

13:30 L. Trifoi *(Concordia University):* Facile Supramolecular Strategy to Construct Solid Fluorophore@Metal-Organic Framework Composites

13:45 L. Wei *(Concordia University):* Molecular copper(I) photosensitizer and cobaloxime photoelectrocatalyst for proton reduction

14:00 L. Miller *(Concordia University):* Electrochemical Analysis of a Ce(IV) UiO Series of Metal–Organic Frameworks

14:15 C. Kaur *(University of Ottawa)* : Antioxidants as a potential solution for oxidative degradation of supported amine materials

Talk Session C // 15:45 – 17:45 (EST)

Analytical & Environmental — SP 265.29

15:45 P. Sojoudi *(Simon Fraser University):* Differentiation of ginseng DNA strands using a Nucleic Acid Lateral Flow Assay (NALFA)

16:00 S. Vij *(Carleton University):* Enhancing the MS-based sensitivity of phosphopeptides by Trimethylation Enhancement using Diazomethane (TrEnDi)

16:15 K. Yeadon *(Carleton University):* Cyclic voltametric analysis of ice formation on surface coatings toward prevention of safety hazards in the aerospace industry

16:30 O. Zambito *(Université du Québec à Montréal):* Multi-omic analysis of Hirschsprung's disease in a mouse model

16:45 J. Osagu *(Concordia University):* Non-targeted screening of organic compounds of potential concerns in urban aquatic environment

17:00 Y. Mirzaei *(Concordia University):* A Kinetic Study on the Degradation and Biochemical Fractionation of Organic Matter in the Biggest Semi-Enclosed Estuary System of the World: an Isotopic and Genomic Approach

17:15 A. Hamilton *(Concordia University):* Lignin-derived heterogeneous catalyst for biodiesel synthesis

17:30 C. Johannessen *(Concordia University):* Monitoring of select tire-derived organic chemicals in urban air

Biochemistry — RF 335

15:45 V. C. Cabana *(Université du Québec à Montréal):* AlphaFold predicts functional protein-protein interaction

16:00 A. Piercey *(McGill University)* : A Series of Controlled Movements Mediate Enzyme Activity: Conformational Dynamics in Cytochrome P450 Reductase

16:15 A. Van Kessel *(McGill University):* Live-cell imaging reveals impaired detoxification of lipid-derived electrophiles is a hallmark of ferroptosis

16:30 W. Zhang *(McGill University):* Investigating Lipid Peroxidation Cell Death via a Fluorogenic Tocopherol Analogue Probe

16:45 C. Bousch *(Université de Montréal):* Synthesis of a fluorogenic photocrosslinker probe to capture glycan-protein interactions

17:00 H. X. Lee *(University of Northern British Columbia):* Small Molecule Growth Inhibitors from Onnia tomentosa Native to British Columbia

Organic Chemistry SP 457.03

15:45 A. Paquette *(University of Ottawa):* Total and Chemoenzymatic Synthesis of Seongsanamide E

16:00 M. Petit *(Université de Montréal):* Development of new antimicrobial agents based on bis-benzimidazolium salts to combat bacterial resistance

16:15 S. Pilavdjian *(Concordia University):* A Three-Pronged Approach to Design Anillin-Specific Inhibitors and Liver Cancer Treatment

16:30 K. Reznikov *(Dalhousie University):* Molecular Characterization of Boron Heterocycles as Biologically Active Compounds

16:45 K. M. Tam *(McGill University):* Electrochemical Palladium-Catalyzed Carbonylation: Oxidation State Shuffling as a Catalyst Design Tool

17:00 P. Prevost *(Concordia University):* Repurposing Drug-Like Molecules for Applications Against Gram-Negative Bacteria through Chemical Modifications

17:15 E. Walsh *(University of Ottawa):* Optimizing alkylated ammonium-based compounds to improve ice recrystallization inhibition (IRI) and cryopreservation efficacy

Computational Chemistry RF 320

15:45 T. Franca *(INRS):* Searching for repurposed inhibitors of ricin through molecular modeling techniques

16:00 J. Genzling *(McGill University):* VIRTUAL CHEMIST or computer-aided design in asymmetric catalysis

16:15 S. Montero Vega *(Carleton University):* Interaction Between Antimicrobial Peptide Magainin 2 and Non-lipid Components in the Bacterial Outer Envelope

16:30 M. Shamekhi *(Concordia University):* High-throughput screening and DFT characterization of bimetallic alloy catalysts for the nitrogen reduction reaction

16:45 N. T. P. Tu *(Carleton University):* MLXDM: Extends Neural Network Potential to Describe Long-range Dispersion Interaction

17:00 N. Kooner *(Concordia University):* Structure, Dynamics, and Oligomerization of Host Defense Peptides: Elucidating the Effect of Charge, Hydrophobicity, and Chirality Using Atomistic Biomolecular Simulations

Nanochemistry

RF 324

15:45 N. Calvert *(University of Ottawa):* Highly NIR-II Scattering Gold Superclusters for Optical Coherence Tomographic Molecular Imaging

16:00 B. Malile *(York University):* Exploring Manganese (II) Doped CdS Quantum Dots for Enhanced Photoredox catalysis

16:15 M. Creran *(Université de Montréal):* Additive Manufacturing of Photoactive Materials

16:30 S. L. Maurizio (*Concordia University):* The effect of host material on lanthanide-doped radioluminescent nanoparticles

16:45 K. Kroeger *(Concordia University):* Phospholipid bilayers as a platform for photoactivated delivery of antimicrobial peptides

17:00 F. Yarur Villanueva *(University of Toronto):* Binary Metal Chalcogenide Templates Direct the Formation of Lead-Free Quaternary Nanocrystals

17:15 M. Kaur *(Concordia University):* Covalent IR820-COOH embedded in dense silica shell around LnUCNPs for NIR dye sensitized based Photocatalysis

17:30 A. Setayesh *(Concordia University):* One-pot Synthesis and Characterization of Chiral Carbon Dots using Response Surface Methodology and Their Anti-bacterial Properties

Poster Session 1 // 10:00 – 12:00 (EST)

Inorganic Chemistry

I01 - E. Brun *(University of Ottawa):* Evaluation of hetero-bislanthanides complexes for MRI and optical imaging

I02 - X. A. Canales Galvez *(Concordia University):* Synthesis of Tb(III)-UiO-66 Analogues with Enhanced Photoluminescence

I03 - C. Copeman *(Concordia University):* Adsorptive Removal of Oxyanions from Water using a Zr-based Metal–Organic Framework

I04 - A. MacKay *(Concordia University):* Solvent-Free Aerobic Oxidations of Phenols by Copper-Based Catalysis

I05 - A. Muhammad *(Concordia University):* Recycling and Reuse of Solvents for the Synthesis and Purification of Metal–Organic Frameworks

I06 - T. Rutherford *(Concordia University):* Electrochemical deposition and conversion of aragonite microstructures into shape-preserving photocatalytic perovskites

I07 - N. Zeinali Galabi *(McGill University):* Accelerated Development of High Voltage Li-Ion Cathodes

Organic Chemistry

O02 - B. Bueno (*Université du Québec à Montréal):* Synthesis of 1-Methylcyclopropyl Aryl Ethers from Phenols using an Alkenylation-Cyclopropanation Sequence

O03 - K. Burchell-Reyes *(Université Laval):* Enantioselective transformations of prochiral α-CF_3 and α-SF_5 ketones

O04 - Z. Zhong *(Concordia University):* Chiral amplification of the conglomerate crystal with temperature control

O05 - E. Delaire *(INRS):* A Medicinal Chemistry Perspective on Fragment-Based Drug Discovery from Hit to Lead

O11 - O. Thibeault *(Université Laval):* Aldehydes Deoxofluorination Using XtalFluor®

Biochemistry

B01 - I. Ajala *(Université du Québec à Montréal):* Subcellular localization and membrane topology of AltSLC35A4, a highly conserved alternative protein among vertebrates.

B09 - A. Montulet *(McGill University):* Diversifying chemical modifications on ASOs promoting exon 51 skipping for Duchenne Muscular Dystrophy

B11 - J. Plamondon *(Université du Québec à Montréal):* Effects of SUMOylation on protein-protein interactions: development and application in Rett syndrome

B12 - C. Quintero Arias *(Trent University):* Gelsolin aggregation and inhibition: Biophysical characterization

B13 - L. Sinnathurai *(Université du Québec à Montréal):* La SUMOylation des facteurs du chocs thermiques (Hsfs) chez *Arabidopsis thaliana*

B14 - M. St-Aubin *(Université de Montréal):* Activity and inhibition of trimethoprim resistant enzymes: insights into evolutionary origin

B15 - A. Sénécal *(Université du Québec à Montréal):* Implementation of the proximity biotinylation approach (BioID) to identify protein complexes associated with RNF13

B16 - I. Tiaiba *(Université du Québec à Montréal):* The role of the SLC35A4 gene in the Integrated Stress Response.

B17 - S. Torabidastgerdooei *(Université du Québec à Montréal):* Metabolic reprogramming reveals a role for the G6PC3 and solute carrier family 37 SLCA2 / SLCA4 components upon the acquisition of a brain cancer stem cell molecular signature

B18 - D. Valdez *(Concordia University):* Identification of selective glycosyltransferase inhibitor molecules targeting cell-surface fucosylation

B19 - N. Weerasinghe *(McGill University):* Investigation of the unique structural elements and catalytically important dynamic regions of the Nisin biosynthetic enzyme NisC

Nanochemistry

N04 - S. Faiad *(McGill University):* DNA-based Strategies for Effective Therapeutic Delivery

N05 - P. Islas *(McGill University):* Automated Assembly of DNA Wireframe Nanotubes Characterized via Single-Molecule Fluorescence Microscopy

N02 - J. Asohan *(McGill University):* Design and Characterization of Self Assembled Spherical Nucleic Acids for Gene Silencing

Poster Session 2 // 18:00 – 19:45 (EST)

Analytical Chemistry

A01 - S. Ghaffari *(York University):* CE to the ReSQ! Automated label-free capillary electrophoresis (CE) analysis of Asparaginase activity using the “Inject-Mix-React-Separate-and-Quantitate” (IMReSQ) Method

A02 - S. Matar *(Université du Québec à Montréal):* In vitro metabolism of BPA analogs by LC-HRMS/MS

Physical Chemistry

P01 - G. Amato *(Concordia University):* Chirality Induced Spin Selectivity in Contact Electrification

P02 - G. Merino *(McGill University):* The formation of protein fibers from Tobacco Mosaic Virus (TMV) self-assembling capsids.

P03 - P. Taktikakis *(Concordia University):* A Comparison of the Physicochemical Impacts of E-Cigarette Additives α-Tocopherol and α-Tocopherol Acetate on Pulmonary Lung Surfactants

Organic Chemistry

O01 - K. Basran *(McGill University):* Mechanistic insight into formal [4+2] cycloadditions of maleimides on duplex DNA.

O06 - V. Mastalerz *(Université Laval):* Synthesis of pentafluorosulfanylated organic compounds by Kolbe-type decarboxylative electrochemical cross-coupling

O07 - A. Mikov *(McGill University):* Synthesis of Trioxoazatriangulene-Based Covalent Organic Frameworks

O08 - M.-R. Ouellet-Du Berger *(Université Laval):* Blacklight-mediated chloropentafluorosulfanylation of alkenes and alkynes

O09 - A. Pontarelli *(Concordia University):* Arabinonucleic Acids Containing C5-Propynyl Modifications Form Stable Hybrid Duplexes with RNA that are Efficiently Degraded by E. coli RNase H

O10 - F. Rémy *(Université Laval):* Synthesis of (2-fluoroallyl)boronates from gem-difluoropropenes

Molecular Biology

M01 - H. Barber *(McGill University):* Chemically Modified Antisense Oligonucleotides Targeting the C9orf72 Repeat Expansion Found in Amyotrophic Lateral Sclerosis

M02 - K. Bietar *(McGill University):* Effects of lanthanide-doped upconverting nanoparticles on nuclear homeostasis

M03 - S. Chu *(McGill University):* Cellular senescence stabilizes microtubules in intestinal epithelial cells

M04 - M.-E. Roy *(Université du Québec à Montréal):* A role for the JAK/STAT signaling pathway in mesenchymal stromal/stem cells vasculogenic mimicry.

M05 - J. Sicheri *(Concordia University):* Yellow is the New Green: Evolution of Old Yellow Enzymes for Sustainable Polymer Production

M06 - K. Skaik *(McGill University):* Investigating the interplay between AMPK and ERK signaling pathways.

M07 - K. Zhao *(McGill University):* Novel fluorogenic DNA intercalators for DNA labeling in living cells

Biochemistry

B02 - J. Brazeau-Henrie *(University of Ottawa):* Studying TE-mediated macrocyclization control mechanism via saturated mutagenesis of the DEBS-TE.

B03 - R. Dupuis *(Concordia University):* LC-MS Analysis of Changes in Cranberry Flavonoids in Crops Grown with Endophytes

B04 - J. Gagnon *(INRS):* Assessing target engagement of newly discovered protein RAS binding compounds using cellular thermal shift assays (CETSA).

B05 - A. Harake *(Université du Québec à Montréal):* Sumo E3 Ligases identification and characterization through bioinformatics

B06 - S. Kaviani *(McGill University):* Sequence-Controlled Spherical Nucleic Acids: Gene Silencing, Encapsulation and Cellular Uptake

B08 - C. Lima *(Université du Québec à Montréal):* Development of a study strategy of N-glycosylated proteins composing human tears by LC-MS/MS

B10 - S. Peslherbe *(McGill University):* Elucidating the structural dynamics and modification mechanism of Haloduracinβ using Nuclear Magnetic Resonance Spectroscopy

Computational Chemistry

C02 - N. Jodaeeasl *(Concordia University):* Towards Rapid Computational Screening of Metal-Organic Framework Candidates for Chemical Adsorption of Small Toxic Molecules

C03 - R. Sulaimon *(Concordia University):* Towards Repurposing of Prescription Drugs as Potential Inhibitors of Botulinum Neurotoxin Metalloprotease

Nanochemistry

N01 - A. Al-Feghali *(McGill University):* From Structure to Function: Bottom-up Fabrication and Individual Characterization of Metamaterials with Resonances in the Visible Regime

N03 - T. Das *(McGill University):* Barcoding DNA Nanostructures for High Throughput Cellular Uptake Studies

N06 - A. Nizami *(Concordia University):* Catalytic Conversion of Polysulfides by Atomic Layer Deposited Titanium Nitride for High-Rate Lithium Sulfur Batteries

Polymer Science

PS01 - N. Chelfouh *(Université de Montréal):* Apple Pectin based Hydrogel Electrolyte for Energy Storage Applications

PS02 - J. Chen *(Université de Montréal):* Polymer Matrix Mediated Assembly of P3HT Nanowires

PS03 - T. Perodeau *(Université de Montréal):* Understanding solid polymer electrolytes through hot melt extrusion additive manufacturing

PS04 - O. Roy *(Université de Montréal):* Development and Optimization of Highly Reflective Electrospun Poly(oxymethylene) Nanofibers

PS05 - R. Zidani *(Université de Montréal):* Polymer additive manufacturing for antimicrobial materials

Abstracts – Oral Presentations

ANALYTICAL CHEMISTRY

Heart Cutting from a Capillary Array

D. Boivin
Concordia University

High resolution capillary electrophoresis (HRCE) is capable of preforming separations of complex samples all while consuming small amounts of buffer. CE, however, does not innately posses the ability to identify the newly separated peaks. An additional method would be needed to overcome this limitation. Off-line fractional collection of peaks is both labour intensive and problematic. The pL peaks volumes make manual sample manipulation impractical. An automated in-line collection technique was developed to address this challenge. We present our “Peak Picker” which collects peak(s) of interest across an array of varied length capillaries onto a single receiver capillary. The Peak-Picker utilizes a sheath-flow interface with the aid of a 3-axis motor-controlled stage to collect peaks as they elute out. The loaded Peak-Picker can then be interfaced with additional analytical instrumentation such as a mass spectrometer for real-time, in-line identification. We demonstrate that the combination of a motorized stage and a sheath-flow interface can reliably facilitate the transfer of peaks from the separation capillaries to the receiver capillary. Experiments in separating and selectively collecting a peak from a mixture of labelled biomolecule standards is ongoing and will be discussed.

Longitudinal LC-HRMS oxylipin profiling to investigate the atherogenicity of low carbohydrate - high protein diets

L. Cougnaud*, A. St-Amant, A. Bergdahl, D. Vuckovic
Concordia University

Oxylipins are signaling lipid mediators involved in various inflammatory pathways. However, the accurate measurement of oxylipins is challenging and requires a large plasma volume, typically 100-1000 µL. The objective of this study was to develop a method compatible with the use of 15 µL of plasma and to apply this method to investigate early atherosclerosis development in ApoE knockout mice. Male mice (n=12) were fed with Low carbohydrate-high protein (LCHP), western, or chow diets with or without probiotic administration (*L. helveticus* and *B. biffidum* at 0.5 and 5 CFU/day). Plasma samples collected at 1, 3, and 5 weeks were extracted using a C18 SPE. LC-MS analyses were performed on an Agilent UHLPC system coupled to a quadrupole time-of-flight using 40-min C18 LC method. The final method covered 72 oxylipins, of which a total of 25 were routinely measured across all samples with good method precision (RSD < 20% for spiked internal standards). Additionally, 10 unknown oxylipins were also measured. Both diets and probiotics affected oxylipins derived from linoleic acid. Furthermore, both western and LCHP diets showed a decrease in eicosapentaenoic and docosahexaenoic acid levels. To conclude, we successfully developed a low-volume method for monitoring oxylipin profiles suitable for longitudinal monitoring.

Metabolome coverage from targeted and untargeted methods

N. Ghafari*, L. Sleno
Université du Québec à Montréal

Metabolomics aims to study the variation of metabolites in biological samples. The understanding of metabolic variation is an important step towards a better understanding of diseases and environmental perturbations. Metabolic changes caused by external or internal stimuli often occur before clinical signs appear. To study the metabolic variations of different biological samples, a "ready to use" commercial kit is being tested to access more than 600 metabolites. The samples are prepared with a derivatization process by phenyl isothiocyanate, followed by protein precipitation and targeted and quantitative LC-MRM analysis on a triple quadrupole platform. To increase metabolic coverage, an untargeted high-resolution tandem mass spectrometry method was also developed on a quadrupole-time of flight platform. To validate metabolite identification from this untargeted data, an in-house spectral library was built from the analysis of over 200 metabolite standards. This presentation will contrast the advantages of both targeted and untargeted approach in a few different biological sample types, including zebrafish and C. elegans.

Rational design of quantum dot surface chemistry for protease detection

K. Krause*, K. Rees, R. Higgins, T. Jeen, R. Algar
University of British Columbia

Proteases play a vital role in human health; there is thus demand for robust assays to detect abnormal protease activity for disease diagnosis. Quantum dot (QD)-peptide conjugates have been used extensively for protease detection. While QD surface chemistry is known to impact protease activity, the mechanisms by which the QD surface affects different proteases are not yet fully understood. Here, we present a systematic survey of QD surface modifications—including rationally designed ligands and regulatory peptides—and their impact on protease activity. A series of small-molecule and polymeric ligands were developed to selectively accelerate, decelerate, or inhibit a range of proteases. Regulatory peptides enable further tuning of QD-protease interactions. We used these strategies to develop a QD-based sensor array capable of differentiating a series of related proteases. Sensor arrays are alternatives to conventional sensors in which analytes are detected and categorized based on

patterns of responses from a series of non-specific sensor elements. We developed a sensor array in which sensor elements consist of QD-peptide conjugates with different combinations of ligands, substrate peptides, and regulatory peptides. This work is a significant advancement in understanding QD-enzyme interactions, where the sensor array is a practical implementation of this understanding.

Stability of oxylipins stored on biocompatible solid-phase microextraction (SPME) devices.

O. Kuteyi*, D. Vuckovic
Concordia University

Oxylipins may degrade during sampling, transportation, and storage, making their accurate measurement in biological specimens extremely challenging. In vivo solid phase microextraction (SPME) is an extraction technique that was recently introduced for the quantification of oxylipins in brain tissue. These devices do not co-extract proteins from the sample, thus eliminating the enzymatic degradation of oxylipins. The aim of this study was to investigate the on-device oxylipin stability to non-enzymatic degradation during the freeze-and-thaw process and at room temperature storage for 18 days. 53 oxylipins were extracted using HLB SPME devices from standard or human plasma samples. To evaluate stability, all tested conditions were compared against control samples (t=0) using the acceptance criteria of within 80-120% and ANOVA statistical analysis. 13- and 11-hydroxy-docosahexaenoic acids were unstable in plasma, whereas 5-hydroxy-eicosapentaenoic acid was unstable in both standard and plasma samples during the freeze-and-thaw experiment. Only 4-hydroxydocosahexaenoic acid was unstable during the room temperature study. The degradation pathways of Identified unstable oxylipins were further investigated using forced degradation studies at 37°C, 50°C and UV exposure at 365 nm. This is the first time the oxylipin stability on SPME devices has been characterized and shows how SPME can successfully improve their stability during storage.

Discovering protein biomarkers for ocular mucous membrane pemphigoid in human tears

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[1]Université du Québec à Montréal, [2]Centre hospitalier de l'Université de Montréal

Mucous membrane pemphigoid (MMP) is a multisystemic rare autoimmune disease affecting different mucous membranes. Ocular involvement is characterized by chronic inflammation of the conjunctiva and abnormal tissue regeneration causing scar formation on the ocular surface. Severe ocular disease leads to corneal opacification resulting in vision loss. Diagnosis by conjunctival biopsy and associated treatments prescribed to prevent scarring can have serious consequences. Following initial untargeted proteomics screening of tear proteins in a healthy population and MMP patients, we have developed a targeted LC-MRM method for a panel of putative biomarkers for diagnosis and routine monitoring of MMP patients. Tear samples were collected on Schirmer strips, and trypsin digested prior to analysis by LC-sMRM method targeting 97 proteins, 20 of which were added to the method for data normalization, on a triple quadrupole platform. This analysis found statistically significant changes between patients with MMP, non-ocular MMP, Lichen Plan (MMP-related disorder) and heathy controls. Biomarker candidates were filtered using a p-value threshold <0.05 and fold change over 2, compared to the control group. This study will contribute to a better understanding of the biological pathways involved in this rare disease and potentially facilitate the diagnosis and staging of this complex disease.

A diagnostic electrochemical aptasensor development for sCD80 protein detection in human serum

A. Malkawi*, M. Jafari, L. Sleno, M. Siaj
Université du Québec à Montréal

Many studies have reported the elevation of soluble CD80 (sCD80) in human serum in different autoimmune diseases such as rheumatoid arthritis. sCD80 level has a potential role in disease development and diagnosis, potentially used as a biomarker for RA. Measuring sCD80 in human serum using immunoassays such as ELISA is associated with different drawbacks, mainly cross-reactivity. Aptamer-based biosensors (aptasensor) development for quantification and detection of different biological molecules is becoming a very popular technique that advances the application in next-generation medicine. Herein, we selected a high-affinity aptamer for sCD80 by the conventional *in-vitro* selection process SELEX. The highest binding-affinity aptamer (K_d = 47.69 nM) was used to construct a sensitive aptasensor on a screen-printed gold electrode (AuSPE) platform associated with label-free electrochemical impedance spectroscopy. The immobilization of the aptamer on the gold surface and the presence of sCD80 in a complex with aptamer were investigated by atomic force microscopy (AFM) and photo-induced force microscopy (PiFM). The developed aptasensor showed a linear performance in the range of 0.025-10 nM of protein with a detection limit of 8 pM. Furthermore, the developed aptasensor was successfully validated using spiked serum samples with the protein, indicating its applicability as a detection tool for sCD80.

LC-HRMS characterization of sulphate and glutathione mycotoxins of 17 mycotoxins found in the Canadian food supply.

E. Mariani*, I. Slobodchikova, C. Zainea, D. Vuckovic
Concordia University

Mycotoxins are toxic secondary metabolites produced by fungi that pose adverse health effects to humans and animals. These toxins are found in foods such as cereals, corn, wine, spices, milk, and eggs. To reduce human exposure, Canada has set regulations for several mycotoxins based on the average daily intake of certain foods. Human biomonitoring studies can be used to verify how well current regulations protect consumer health. However, current biomonitoring methods often do not include mycotoxin metabolites which can significantly underestimate exposure. Therefore, the aim of this study was to produce and characterize sulphate and glutathione metabolites of 17 mycotoxins including aflatoxin, zearelanone, and trichothecene class. Metabolites obtained from Phase II or Phase I + phase II microsomal incubations were characterized using pentafluorophenyl

liquid chromatography-high resolution mass spectrometry (LC-HRMS) on ion trap – Orbitrap instrument. To date, 19 sulphate metabolites and 11 glutathione metabolites were characterized using accurate mass, MS/MS, and MS^3 fragmentation. Among these, nine metabolites were reported for the first time. Furthermore, sulphation reactions were conducted on phase I mycotoxin metabolites to characterize additional 21 minor metabolites. All metabolites were added to an extensive in-house LC-MS library to support future biomonitoring studies.

Evaluation of Ionic Liquids using Dispersive Liquid-Liquid Microextraction for Metabolomics

R. Maulana*, D. Vuckovic
Concordia University

In recent years, ionic liquids (ILs) have emerged as a popular alternative for organic solvents due to their unique properties and customizable cations and anions, dubbing them as designer solvents. Due to their customizability and selectivity, ionic liquids have shown to be effective in extracting biological analytes such as lipids and metabolites. Here, the extraction selectivity of two ionic liquids, 1-hexyl-3-methylimidazolium hexafluorophosphate ($[C_6MIM][PF_6]$) and trihexyl(tetradecyl)phosphonium hexafluorophosphate ($[P_{6,6,6,14}][PF_6]$), was evaluated in dispersive liquid-liquid microextraction (IL-DLLME) format for selected lipids and metabolites. Methanol was used as dispersing solvent. The resulting supernatants were analyzed using liquid chromatography-mass spectrometry (LC-MS). The results showed similar selectivity of $[P_{6,6,6,14}][PF_6]$ and $[C_6MIM][PF_6]$ towards lipid extraction. Future work will further systematically investigate extraction selectivity of these ILs in standards and human plasma and urine.

Semi-targeted LC-HRMS/MS analysis to decipher the effects of acetaminophen on human bile acid profiles.

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Université du Québec à Montréal

Acetaminophen (APAP) is a very common analgesic used worldwide to relieve pain and decrease fever. Unfortunately, when taken excessively, this drug can cause acute liver failure through the formation of its reactive metabolite, N-acetyl p-benzoquinone imine (NAPQI). This reactive species binds to liver proteins leading to liver failure. Previous studies have shown that APAP can interfere with bile acid synthesis and increased levels of circulating bile acids is a marker of liver disease. To investigate the effects of acetaminophen on circulating bile acid profiles, metabolites were extracted from sera of human patients with APAP-related acute liver failure and healthy controls. Bile acids were analyzed by LC-MS/MS and all peaks detectable in samples from a standard mix of 46 bile acids were assigned based on accurate mass and retention time. Then, potential bile acid isomers not contained in the standard mix, as well as putative glucuronide and sulfate conjugates of these bile acids were assessed by accurate mass filtering. Our results showed that acetaminophen significantly influenced the levels of bile acids and conjugates. Several peaks varied significantly between healthy controls and ALF patients, as well as some statistically relevant changes based on patient outcome.

Singlet Oxygen Flux and Membrane Expansion Dynamics Visualized on Giant Unilamellar Vesicles

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Singlet oxygen ($^1O_2$) is one of the most detrimental reactive oxygen species, where its reaction with key biomolecules such as DNA, proteins, and lipid membranes ultimately lead to cellular death. Particularly, its reaction with unsaturated lipids generates lipid hydroperoxides, and leads to the expansion, thinning, and eventual leakage of lipid membranes. Direct detection and quantification of $^1O_2$ in lipid membranes is challenging due to its short lifetime, whereas its accurate indirect quantification through commercially available sensors is still lacking due to competing reaction pathways. Here we use a very sensitive fluorogenic probe, H_4BPMHC, for the real time quantification of $^1O_2$ flux in lipid membranes. Upon its reaction, the probe undergoes an impressive 350-fold emission enhancement that follows zero order reaction kinetics, enabling an easy and reliable method for the quantification of $^1O_2$ flux. We devised microscopy studies that enable the real-time monitoring of the flux of photosensitized $^1O_2$ into giant unilamellar vesicles GUVs and the visualization of the ensuing collective membrane expansion dynamics associated to molecular changes in the lipid structure upon hydroperoxide formation. Together, our imaging studies provide a methodology to explore the intimate relationship between chemical insult, membrane morphology and its collective dynamics.

Chemical Derivatization of Glufosinate via Trimethylation Enhancement Using Diazomethane (TrEnDi) for Enhanced Mass Spectrometry Analysis in Canola Samples

K. Sheedy*, C. Rosales, J. Manthorpe, J. Smith
Carleton University

Glufosinate is one of the most commonly used herbicides worldwide, it inhibits glutamine synthetase which results in increased ammonia levels in plants and mammals. Glufosinate ammonium is sold under many trade names, such as Liberty®, which is commonly used on corn, soybeans, and canola crops. Due to its high polarity, low volatility, small size and lack of chromophores and fluorophores, glufosinate is difficult to detect at trace levels. Using the chemical derivatization strategy trimethylation enhancement using diazomethane (TrEnDi) glufosinate reacts with diazomethane and tetrafluoroboric acid to create a fixed permanent positive charge on the amino group by the formation of a 4° ammonium ion. When using high performance liquid chromatography tandem mass spectrometry (HPLC-MS/MS), analyte retention on the reversed-phase column is increased 3-fold and the sensitivity is increased 4.1-fold in standard solution. TrEnDi methodology was applied to canola samples from two separate fields that were both sprayed with Liberty® in June 2021 and collected before harvest in September of 2021. The

analysis showed there were trace quantities or no signal associated with unmodified glufosinate, however TrEnDi modification resulted in improved and quantifiable signals from permethylated glufosinate.

Differentiation of ginseng DNA strands using a Nucleic Acid Lateral Flow Assay (NALFA)

P. Sojoudi*, P. Li
Simon Fraser University

Panax ginseng (Pgin) and Panax quinquefolius (Pquin), which have different benefits and costs, are hard to be differentiated based just on their appearances especially when they are in powdery form. So, a molecular test that can be used in a commercial setting is required to overcome this. To distinguish between Pgin and Pquin, an SNP site has been chosen on the DS gene. An isothermal nucleic acid amplification test (NAAT) will be developed to directly detect the extracted plant DNA, which will be amplified in situ. A nucleic acid lateral flow assay (NALFA) has been designed which consists of four major components, i.e sample pad, conjugate pad, nitrocellulose membrane which serves as the reaction matrix, and adsorbent pad. A colorimetric detecting NALFA device has been tested based on visual detection due to gold nanoparticles (20 nm). Only when the target DNA of ginseng is present, a red colour spot will appear on the membrane, observable by the naked eye. Two capture probes are designed based on the chosen SNP site and they are complementary to the Pgin and Pquin target sequences. The detection probe has a sequence complementary to the Pgin/Pquin sequences as well as the control sequence.

Enhancing the MS-based sensitivity of phosphopeptides by Trimethylation Enhancement using Diazomethane (TrEnDi)

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Carleton University

Mass spectrometry is regarded as a powerful tool for studying phosphopeptides. However, several challenges are commonly encountered, including difficulties detecting phosphopeptides with low stoichiometry, relatively high hydrophilicity & low ionization efficiency compared to unmodified phosphopeptides. Here we present TrEnDi, a method to improve the analytical characteristics of phosphopeptides. TrEnDi overcomes these challenges & increases the sensitivity via permethylating analytes, rendering them permanently positively charged & eliminating the need for protonation. Synthetic phosphopeptides, FLEEpSK, FLEEpTK, & FLEEpYK, loaded on strong cation exchange chromatographic resin, were derivatized with diazomethane & were analyzed using a mass spectrometer. The derivatization resulted in ~100% complete methylation of the acidic groups on the phosphopeptides, indicated by a mass shift of +154 Da, highlighting the addition of eleven methyl groups. The complete methylation of these phosphopeptides induces fixed positive charges on the N-termini & lysine residues. MS^2 analyses of the phosphopeptides revealed the methylated sequence of each peptide. Reversed phase LC-MS analysis of the TrEnDi modified phosphopeptides revealed a relative increase in retention by 8%, greater separation between species & a five-fold increase in sensitivity for modified phosphopeptides compared to their unmodified counterparts. TrEnDi may be used to boost the sensitivity of phosphopeptides in complex biological samples.

Cyclic Voltametric Analysis of Ice Formation on Surface Coatings Toward Prevention of Safety Hazards in the Aerospace Industry

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[1]Carleton University, [2]NRC Aerospace Research Centre

Ice accumulation on the surface of aircraft is a major source of safety hazards and property damage in the aerospace industry. The predominantly used active ice protection technologies are costly and energy-intensive, so passive options provided by icephobic coatings have been hailed as a greener and more affordable means of deicing aircraft. Ice adhesion values of icephobic coatings are widely reported; yet, icing behaviour at nucleation and during its spread across a surface are not well understood. This research aims to provide novel information about the initial stage of ice formation by determining the exact temperature of ice formation on various surfaces – particularly icephobic coatings – using cyclic voltammetry for electrochemical analysis. By slowly lowering the temperature of a laboratory icing set-up, cyclic voltammograms can be used to continously measure electron transfer behaviour of a redox probe in a water droplet on a surface as it freezes to form ice. The resulting voltammograms have been observed to distort in shape during this phase change allowing us to pinpoint the exact temperature of ice formation. The comparison of these distortions across surfaces of different chemistry under different physical conditions can provide novel information about the initial stage of ice formation.

Multi-omic analysis of Hirschsprung's disease in a mouse model

O. Zambito*, L. Ohlund, C. Toufaily, R. Soret, N. Pilon, L. Sleno
Université du Québec à Montréal

Hirschsprung's disease is a rare disorder affecting nerve cells in the intestine, causing obstruction of the colon from a lack of neural ganglia cells, having an incidence of 1 in 5000 births. Some patients present moderate symptoms such as constipation, while others can develop dangerous infections leading to major complications, including death. The focus of this study is to better understand the metabolic and proteomic perturbations using LC-MS/MS as there are currently still many unknowns related to this disease. This could provide further insight into the development of the disease, as well as provide potential biomarkers for therapeutic assessment. We have conducted an untargeted study to investigate metabolite and protein-level perturbations from colon tissue samples, comparing a mouse model of Hirschsprung's disease and wild-type mice, using liquid chromatography coupled to high resolution mass spectrometry. Currently, we have identified around 40 putative metabolites and 20 proteins, to be examined more closely for their involvement in this disease in follow-up studies. The workflow for sample preparation, analysis and data processing will be described, as well as the results and perspectives for future work.

INORGANIC CHEMISTRY

Antioxidants as a potential solution for oxidative degradation of supported amine materials

C. Kaur*, A. Sayari
University of Ottawa

Supported amines have been extensively studied as promising basic catalysts and as materials for CO_2 capture. However, they are prone to oxidation, which leads to their degradation and shorter lifetime. This is the major drawback of these materials which acts as a barrier for their commercialisation. In this work, we aim to develop methods to increase the oxidative resistance of supported amine materials. Two methods were employed to investigate the impact of amine functionalization and addition of antioxidants on the oxidative resistance of such materials. In the first approach, propylamine was functionalized with glycerol carbonate to introduce hydroxyl groups, whereas in the second method, sulphur-containing antioxidants such as methimazole was dispersed into impregnated polyethylenimine (PEI). Fresh and modified materials were exposed to air at 110 ºC for different time intervals and their CO_2 adsorption capacity was measured by thermogravimetric analysis (TGA) to monitor their oxidative resistance or the lack thereof. Grafted propylamine improved oxidative resistance, while surprisingly, sulphur-containing antioxidants led to further oxidative deterioration. Further investigations of these findings are currently in progress.

High-throughput studies of Li-La-Zr-O garnet solid electrolytes

E. Anderson*, A. Jonderian, E. McCalla
McGill University

Lithium lanthanum zirconium oxide (LLZO) is a leading candidate electrolyte for solid Li-batteries due to its high lithium-ion conductivity, stability in air and against Li metal, and compatibility with high-voltage cathodes. Herein, we have applied a high-throughput citrate sol-gel methodology for synthesizing, characterizing, and testing sets of 64 LLZO electrolytes at the mg-scale. Using our methodology, we have studied over 700 samples to produce a full phase stability diagram for the Li-La-Zr-O pseudoternary system. We find that there is significant solubility of Li into the $La_2Zr_2O_7$ pyrochlore structure commonly found as an impurity in LLZO synthesis. We also find that LLZO appears as both tetragonal and cubic forms throughout the system, with cubic LLZO appearing in an extremely restricted region that is difficult to access as a pure phase due to lithium loss, while excess lithium leads to tetragonal LLZO. Li conductivity measurements show that both cubic and tetragonal undoped LLZO have similar bulk conductivities, but there is only a limited region near the formal $Li_7La_3Zr_2O_{12}$ composition where grain boundary conductivity is high. Our methodology is also applied to a comprehensive doping study where over 50 different dopants are evaluated.

Characterization of a Ferryl=oxoheme form of *Staphylococcus aureus* IsdG

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[1]University of Vermont, [2]AbbVie

IsdG is a heme degrading enzyme in the iron acquisition pathway of Staphylococcus aureus. Unlike canonical heme oxygenases, S. aureus IsdG catalyzes the conversion of heme to staphylobilin and its mechanism still remains obscure. A ferryl=oxoheme species with a hydroxylated porphyrin is a critical intermediate for the IsdG-catalyzed reaction. A comparatively long lived, spectroscopically-unique, analogue of this species named Compound X, is formed after reaction of heme-bound IsdG (IsdG–heme) with 10 equivalents of meta-chloroperbenzoic acid (mCPBA) and has a half-life of 4.7 min. This species is characterized using UV-Vis absorption (Abs), magnetic circular dichroism (MCD) and electron paramagnetic resonance (EPR) spectroscopies along with isotopic labeling. The geometric and electronic structure of compound X was modeled using hybrid quantum mechanics/molecular mechanics (QM/MM) and time-dependent density functional theory (TDDFT) calculations. The spectroscopic and computational data revealed that compound X is a ferryl=oxoheme containing a Trp-based cation radical. The detailed characterization, implications of these findings with respect to the enzymatic mechanism of IsdG, and the electronic structures of ferryl=oxohemes in general, will be discussed.

Combinatorial Study of Systematic Aluminum Substitution into NMC Cathode Materials

A. Hebert*, E. McCalla
McGill University

Li-ion batteries power our modern mobile world. They are already used in billions of devices and are powering more of our transportation every day. The cathode material in Li-ion batteries is the limiting factor in terms of battery capacity, as well as one of the culprits leading to battery failure. Thus, improving the cathode material is critical. The layered metal oxides $LiNi_xMn_yCo_{1-x-y}O_2$ (NMC) are the current market leaders in the cathode space. Many compositions are in use with a strong drive toward higher energy by increasing nickel content. However, high-Ni compositions come at the cost of material stability, which impacts battery lifetime. To stabilize the cathode, many metals have been substituted into the material to resist material degradation. However, most studies are limited to substitutions into a few compositions of NMC. In this work, the effects of different levels of aluminum substitution are investigated by preparing 320 different materials using high-throughput methods and characterizing them with both X-ray diffraction for structural characterization and high-throughput electrochemical techniques to extract battery metrics. This work provides insight into the extent to which different NMC compositions accommodate aluminum and the effects on their performance.

Hybrid Inorganic Perovskite-Photonic Crystal Beads with High Quantum Yields of Photoluminescence

V. Lapointe*, M. Majewski, S. Chegadu, M. Ganesh, C. Pomilio
Concordia University

The integration of photonic materials with semiconductor nanocrystals by correlating the photonic stop band and bandgap energy is expected to afford hybrid materials with enhanced optoelectronic properties. Here, we report two photonic crystal–perovskite nanocrystal microbead hybrids synthesized through simple vacuum drying techniques. Polystyrenemicrobeads combined with metal halide perovskite ($CsPbBr_3$ and $CsPbBr_xCl_y$) nanocrystals yield a hybrid with an expected photoluminescence peak when excited above the bandgap energy but an unexpected average photoluminescence quantum yield (as high as 198 %) representing quantum yields that are two- to three-fold higher than the parent nanocrystal materials. These microbead hybrid systems also demonstrated better resistance to degradation in water over 30 days of immersion as compared to their colloidal counterparts.

Electrochemical Analysis of a Ce(IV) UiO Series of Metal–Organic Frameworks

L. Miller*, A. J. Howarth
Concordia University

Metal–organic frameworks (MOFs) have potential in a variety of applications from sensing to catalysis to energy storage devices. The archetypal MOFs Zr-UiO-66 and Zr-UiO-67 are some of the most well studied MOFs, though the study of rare-earth (RE) analogues of UiO-66 and UiO-67 is still in its infancy. The use of rare-earth (RE) ions in MOFs is particularly relevant to modern chemistry due to their large abundance in the earth's crust. Among REs, the most abundant is cerium, which is also one of the few REs to commonly be found in more than the singular +3 oxidation state as it can easily be oxidized to the +4 state. This simple redox property has previously been utilized for organic transformations with Ce(IV) as an oxidizer and this shows great potential for MOFs containing Ce(IV) ions. While Ce(IV)-UiO-66 and Ce(IV)-UiO-67 have been studied for a few general organic catalytic reactions, herein the effect of functionalizing the organic linker of the MOFs on their stability and redox activity is explored. Analysis of the fundamental properties of these electrochemically active MOFs contributes to the reticular design of these materials and to the fast-growing database of applications in energy storage, sensing, and catalysis.

Thiolated Metal–Organic Frameworks for Ophthalmic Drug Delivery

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Cataracts are one of the leading causes of vision loss resulting from the clouding of one or both lenses of the eyes due to protein aggregation. Eye drops provide a simple and non-invasive method for drug delivery but drug penetration to the intended target is limited due to the anatomy and physiology of the outermost layers of the eye. Hence, the focus of this research is to develop a better shuttle for ophthalmic drug delivery providing slow and sustained release of the drug to the intended target while decreasing the frequency of drug administration required. Metal–organic frameworks (MOFs) are a class of porous and crystalline structures comprised of metal nodes bridged by multitopic organic linkers. Owing to their high modularity, tunable pore sizes, and high surface areas, they are promising drug vectors for applications in drug delivery. Herein, a series of Zr-based MOFs are explored as drug vectors for ophthalmic drug delivery. The synthesis and characterization of the MOFs, as well as mucoadhesive properties, and drug loading and release behavior will be discussed.

Rare-earth metal–organic frameworks with a pyrene-based linker for the photo-oxidation of a sulfur mustard simulant

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Metal–organic frameworks (MOFs) are materials comprised of metal clusters, interconnected by multitopic linkers giving rise to a crystalline porous structure. MOFs have been studied for their potential application in gas adsorption, sensing, catalysis, and others. Transition metals are often applied in MOF synthesis, however, rare earth (RE) metals, which include scandium, yttrium, and the series of fifteen lanthanoids, have also been explored due to the intricate topologies and specific properties that RE-MOFs can feature. This work exposes the synthesis and characterization of an isostructural series of RE-MOFs obtained using a tetratopic pyrene linker (H_4TBAPy) and named RE-CU-10 (RE = Y (III), Gd (III), Tb (III), Dy(III), Ho(III), Er(III), Yb(III), Tm(III), Yb(III) and Lu(III); CU = Concordia University). RE-CU-10 shows an **shp** topology, which originates from 12-connected RE_9-cluster secondary building units (SBUs), with D_{6h} symmetry, and 4-connected linkers, featuring 1D triangular channels and cages. The accessible surface area and the ability of the pyrene linkers to generate singlet oxygen under ultra-violet (UV) irradiation, make RE-CU-10 a good candidate for the selective photo-oxidation of the sulfur mustard simulant 2-chloroethyl ethyl sulfide (2-CEES). The synthesis, characterization, and photo-oxidation performance will be discussed along this new series of RE-MOFs.

Microstructured Semiconductor Surfaces Towards Enhanced Light Harvesting for Dye-Sensitized Photocatalytic Systems

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Through the tailoring of semiconductor surfaces, favourable photocatalytic properties are obtained and tuned. Herein, the slow photon region of photonic materials is utilized for increased photon absorption by a photosensitizer, enhancing the efficiency of photocatalytic reactions. Through the introduction of repeating microstructures in a semiconductor, a constructive/destructive interference pattern is generated, resulting in a photonic stop band, which traps and guides light throughout the structure. By

altering the lattice spacing of the repeating structure, light of a target wavelength is selectively trapped. Matching this trapped light to the absorbance profile of a photocatalyst/photosensitizer anchored to the semiconductor surface leads to improved photocurrents and catalytic efficiency. In turn, it is possible to produce photocatalytic films with a reduced loading of potentially expensive catalysts. Furthermore, the porous nature of the photonic material results in an increased surface area on which the photosensitizer is anchored, and for electron transfers to occur. By coupling the favourable properties of photonic structures with accessible synthetic methods, inexpensive and simple to use devices are obtained, resulting in an increased potential for scalability. In this work, photonic systems of varying microstructure sizes are explored and coupled to Cu(I)bisdiimine photosensitizer complexes, and the optimal size is determined.

Facile Supramolecular Strategy to Construct Solid Fluorophore@Metal-Organic Framework Composites

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Fluorescence microscopy enables the visualization of complex biological systems and processes. However, the utilization of organic dyes as bioimaging agents presents several challenges such as stability in biological environment, reduced photostability, and lower quantum yields. Substantial effort has gone into the improvement of the photophysical properties of biocompatible fluorescent molecules (fluorophores). We have designed and fabricated a supramolecular nanosystem consisting of a highly emissive fluorescein derivative encapsulated within the zeolitic imidazolate metal-organic framework, ZIF-8. Confinement of the fluorescein inside the MOF leads to increased dye photostability and quantum yield, longer lifetime, and better organization of the chromophores, meanwhile providing a convenient solution to issues related to scarce solubility or aggregation induced quenching (AIQ) phenomena. Furthermore, post synthetic functionalization of the nanostructures with targeting agents can direct precise accumulation within cells. In principle, this simple protocol can evolve into a general strategy to deliver intracellularly functional molecular components for targeted bioimaging applications.

Molecular copper(I) photosensitizer and cobaloxime photoelectrocatalyst for proton reduction

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Previously, our group has shown that a copper(I)-based donor-chromophore-acceptor molecular system immobilized on a zinc oxide photoanode together with a copper(II)-based water oxidation catalyst can act as a light-harvesting photocatalytic assembly to split water. To enable the complementary reaction to reduce the protons formed from water splitting, we have designed a photocathode comprised of a copper(I)-based chromophore-acceptor dyad complex to drive a well-studied cobaloxime hydrogen evolving electrocatalyst with visible light. In this work, this dyad complex will be installed on fluorine-doped tin oxide glass with a nickel oxide film and will work in concert with the previously studied photoanode to give a tandem cell where hydrogen gas as a solar fuel is expected to be produced effectively. This presentation will outline our present efforts towards this final device, highlighting the synthesis and characterization of the molecular components as well as preliminary investigations of the photocathodes.

PHYSICAL CHEMISTRY

Phosphole-lipid films: 2D self-assembly, head group interactions, and external effects

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Heteroatom-doped p-conjugated systems have been of interest for the design of electronic devices. The presence of phosphole and the partial overlap of phosphorus lone pair with the backbone π orbitals in these systems can influence photophysical, redox, or charge transfer properties. The self-assembly of these systems can be manipulated by introduction of lipid chains and chemical modification of the phosphole head-group. The electrostatic interactions can further be controlled by variation of the counter-ion. Lipids with phosphole-based head-groups have been designed and show intramolecular conformational changes in response to external conditions. The electronic and amphiphilic character of these phosphole-lipids results in hydrogen bonding, π-π interactions, and powerful ionic interactions. In this work, we explore the interfacial self-assembly of a triple-chain phosphole-lipid at air-liquid and air-solid surfaces. The structural organization of these monolayers are studied using surface tensiometry, Brewster angle microscopy (BAM), and imaging ellipsometry. The film morphology of deposited films is visualized using atomic force microscopy (AFM). The phase behavior is evaluated to probe the role of intermolecular π-π interactions and electrostatic interactions on film organization and stability. We also investigate film response to ion adsorption from the subphase to assess their impact on the self-assembly of the phosphole-lipid.

A novel bulky P-dopant for organic semiconductors

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The p-doping of organic semiconductors (OSC), that is conjugated organic molecules (COMs) and polymers (COPs), is generally 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 COP/COM and the p-dopant. Common dopants of high EA (> 5 eV) are typically light-weight, unstable, show low solubility in common solvents with most COPs/COMs, and tend to diffuse through

the semiconductor host. Furthermore, their planarity can lead to the formation of ground-state charge transfer complexes (CPXs) with the COPs/COMs, which is detrimental to doping efficiency. Recently, a new generation of dopants has been introduced based on a cyclopropane core, such as hexacyano-trimethylene-cyclopropane (CN6-CP) of high EA= 5.87 eV, and trimethyl 2,2′,2″-(cyclopropane-1,2,3-triylidene)-tris(cyanoacetate) (TMCN3-CP, EA= 5.5 eV). However, they are largely unsuitable for practical applications due to instability in solvents, air, and even under an inert atmosphere. Here, we introduce a novel, bulky and non-planar dopant 2,2',2''-(cyclopropane-1,2,3-triylidene)tris(2-(perfluorophenyl)acetonitrile) (3PFP3CN-CP) with EA of 5.07 eV. We have observed remarkable stability of this dopant under an inert atmosphere, and doping experiments reveal the suppression of CPX formation, which occurs with planar dopants such as tetracyanoquinodimethane (TCNQ).

Synthesis of Boroxine and Dioxaborole Covalent Organic Frameworks via Transesterification and Metathesis of Pinacol Boronates

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McGill University

Boroxine and dioxaborole are the first and some of the most studied synthons of covalent organic frameworks (COFs). Despite their wide application in the design of functional COFs over the last 15 years, their synthesis still relies on the original Yaghi's condensation of boronic acids (with itself or with polyfunctional catechols), some of which are difficult to prepare, poorly soluble, or unstable in the presence of water. Here, we propose a new synthetic approach to boroxine COFs (on the basis of the transesterification of pinacol aryl boronates (aryl-Bpins) with methyl boronic acid (MBA) and dioxaborole COFs (through the metathesis of pinacol boronates with MBA-protected catechols). The aryl-Bpin and MBA-protected catechols are easy to purify, highly soluble, and bench-stable. Furthermore, the kinetic analysis of the two model reactions reveals high reversibility (Keq ~ 1) and facile control over the equilibrium. We show the generality of this approach by the synthesis of seven known boroxine/dioxaborole COFs whose crystallinity is better or equal to those reported by conventional condensation. We also apply metathesis polymerization to obtain two new COFs, Py4THB and B2HHTP, whose synthesis was previously precluded by the insolubility and hydrolytic instability, respectively, of the boronic acid precursors.

Superior Photoprotection of Cyanine Dyes with Thio-imidazole Amino Acids to Maximize Photon Budget in Single Molecule Fluorescence Studies

J. Ramos Sanchez*, Y. Gidi, T. Lovell, G. Cosa
McGill University

Photostability is one of the main challenges in single-molecule fluorescence imaging. Triplet states and radicals are long lived reactive species that can lead to photodegradation. Therefore, photostabilizers are necessary to mitigate these processes. Oxygen is known to be an efficient triplet quencher; however, it has been associated with photodegradation. Removal of oxygen may increase the survival time of the fluorophores; however, it causes undesired blinking due to the persistence of long-lived triplet state and radical species. A Reducing and oxidizing (ROXS) strategy has been successfully used to decrease the triplet lifetime. In a ROXS scheme a reducing agent can undergo electron transfer with the fluorophore and the formed radical can be oxidized by a second species to recover the singlet ground state of the dye. Nevertheless, the formed radical can lead to photobleaching if the second reagent is not found fast enough. Thiol-based photostabilizers quickly regenerate the fluorophore ground state and circumvent the need of a second additive; however, currently reported can only efficiently quench Cy3 and induce Cy5 blinking. We show two thiol-based amino acids, ergothioneine and 2-thiol histidine, that markedly enhance Cy3B, Cy5, and Cy5B performance over currently used β-mercaptoethanol. Additionally, unlike other thiols, they avoid Cy5 blinking.

ORGANIC CHEMISTRY

Synthesis of urea-based transporters and their anion transport activity

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Control of chloride's transport across the membrane is a challenging subject due to the intrinsic properties of the cellular membrane. An unbalanced transport of those anions can lead to a variety of diseases, such as cystic fibrosis. In most cases, insertion of synthetic transporters in the membrane can restore chloride's transport by various mechanisms. Our main goal is to synthesize anion transporters, with high specificity towards chloride, whose self-assembly in the membrane bilayer is driven by supramolecular interactions. Amphiphilic urea derivatives have been used as small molecules to transport chloride for over a decade. Our goal is to develop new urea derivatives bearing different ligands to further improve chloride's transport efficiency. Addition of a metal source will promote formation of new supramolecular structures in the membrane using organometallic chemistry as a driving force. Those metallic complexes are opening new avenues in the possible geometry of active synthetic transporters.

Synthesis of Tertiary Alkyl Fluorides by Hydrofluorination of Alkenes and Deoxyfluorination of Alcohols

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Alkenes, being one of the most abundant functional groups, can be used as interesting building blocks for the synthesis of fluorinated molecules. This talk will present a method for the hydrofluorination of alkenes using cheap, commercially available, and easy-to-handle reagents. The use of a methanesulfonic acid/triethylamine trihydrofluoride combination allows for the synthesis of alkyl fluorides in up to 78% yield. By changing the fluoride source for another halogen source, hydrochlorination, hydrobromination and hydroiodination could also be performed. The synthesis of fluorinated compounds from alcohols is a well-known reaction, commonly done with deoxyfluorination reagents, such as DAST, Deoxofluor, or XtalFluor-E. However, the deoxyfluorination of tertiary alcohols remains a challenge due to the ease of elimination. Inspired by our hydrofluorination method, we developed conditions that allow for the deoxyfluorination of tertiary alcohols without the need for a prior derivatization. Tertiary alkyl fluorides are obtained in excellent yields, with no elimination observed.

A Continuous Flow Platform for Photochemical Macrocyclization of Peptides.

O. Bleton
Université de Montréal

Despite the impact of photocatalysis in molecular synthesis, extension to macrocyclization has been limited. The prevalence of high dilution techniques renders photochemical approaches problematic due to poor photon flux. Our group has developed a custom designed reactor which combines aspects of plugflow reactors (PFRs) and continuously stirred tank reactors (CSTRs), affording a hybrid technology capable of improving reaction yields in a macrocyclic oxidative dimerization of thiols. A detailed description of the hybrid reactor system and application to the synthesis of complex macrocyclic polypeptides will be presented.

An Organocatalytic oxy-Cope/Michael Cascade Reaction

D. Campbell*, J. Gleason
McGill University

Our group has discovered a diazepane carboxylate catalyst to accelerate the all carbon cope rearrangement via LUMO-lowering catalysis1. In an effort to extend this rearrangement towards more synthetically valuable targets, our group pursued the oxy-Cope variant, which possess a thermodynamic driving force and sees significantly more use in synthesis. It was envisioned that the final product of the oxy-Cope would not be of that of a simple rearrangement, but one where the resulting enol/enol ether intermediate would further react via a Michael addition to furnish cyclopentane-containing products. The reaction proceeds with a range of 3 - hydroxy and 3– alkoxy-1,5-hexadiene-2-carboxaldehydes substrates, including both cyclic and acyclic substrates, and tolerates substitution on the vinyl substituent in good yield, at ambient temperature with a co acid present. Substrates fused on a cycloalkane framework undergo net ring-expansion/cyclopentannulation with a high degree of stereocontrol via chairlike transition states. This methodology allows quick access into natural products such as isodaucene that contains a 5-7 bicyclic framework and the fusicoccin/ophiobolin families that encompasses 5-8-5 tricyclic skeletons.

Investigating a Macrocyclic Strained 1,3-Diyne in “Click” Cycloadditions.

C. Cruché
Université de Montréal

Strained molecules are useful tools in chemistry. Often referred to as “spring-loaded molecules”, release of strain energy or tension can help promote quick and efficient transformations. Strain-promoted alkyne-azide cycloadditions, or SPAACs, have found myriad applications in biolabelling where they obviate the need for toxic copper catalysis. Cyclooctynes and benzocyclooctynes have been developed for in-vitro imaging, but suffer from lengthy and cumbersome syntheses, low stability for prolonged storage and as a result, high commercial costs. Our group has explored a new type of strained molecule for analogous “Click” reactions based on a [1,1':3',1']**trip**henyl macrocyclic skeleton embedded with a bent 1,3-**diy**ne (**TPDY**). An expedient synthesis in three steps and reactivity in different Click reactions will be presented.

Synthesis of a constitutional isomer of armeniaspirol A, pseudoarmeniaspirol A, via Lewis acid-mediated rearrangement

M. Darnowski*, C. Boddy
University of Ottawa

The natural product armeniaspirol possesses a unique spirocyclic N,O-ketal in an α,β-dichloro-α,βunsaturated lactam scaffold that has proved challenging to synthesize. Herein we characterize the oxidative chlorination of pyrrole-2-carboxylate derivatives that rapidly generates this scaffold. The scope of this oxidation was extended to a series of esters and amides. Pyrrole-2-ketones could not be converted into the lactam due to an oxidative fragmentation. This result was unexpected since chloroarmeniaspirol has been synthesized via oxidative chlorination of a pyrrole-2-ketone. Examination of this successful oxidation showed the desired scaffold was accessed due to intramolecular trapping from the neighboring free phenol, preventing fragmentation. Using the product of methyl N-methyl pyrrole-2- carboxylate oxidation, we attempted to access the natural product armeniaspirol, however an unanticipated Lewis-acid mediated rearrangement led to formation of a constitutional isomer, pseudoarmeniaspirol A. A small panel of pseudoarmeniaspirol analogues were synthesized and evaluated for antibiotic activity, inhibition of the targets of armeniaspirol, ClpXP and ClpYQ, and protonophore activity. While pseudoarmeniaspirol shows antibiotic activity, it does not target ClpXP or ClpYQ and has less protonophore activity than the natural product.

Development of Small-Molecules TEAD Inhibitors Derived from Flufenamic Acid

A. Fnaiche
Université du Québec à Montréal

The Hippo pathway regulates organ size and tissue homeostasis by controlling cell proliferation and apoptosis via the YAP–TEAD transcriptional complex. Dysregulation of the Hippo pathway in cancer cells results in the over expression of genes that regulate cancer cell growth and proliferation. Recently, flufenamic acid (FA) was reported to bind in the TEAD palmitic acid pocket, leading to reduction of the expression of associated oncogenes. In this talk, I will present our investigations into the replacement of the trifluoromethyl group of FA by aromatic groups, leading to compounds with increased affinity for TEAD. The impact of these compounds on the activation and expression of TEAD-associated genes will be presented and a docking model will be proposed to explain the binding mode of these compounds.

Gold-catalyzed hydrofluorination of alkynes using hydrofluoric acid

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The gold-catalyzed hydrofluorination of alkynes represents a straightforward and practical method for the synthesis of monofluoroalkenes. All the systems initially developed use an amine- or a urea-complexed hydrogen fluoride as the HF source. Recently, we reported the Au-catalyzed hydrofluorination of internal alkynes using hydrofluoric acid. Both symmetrical and unsymmetrical internal alkynes could be utilized. However, terminal alkynes reacted mostly with water to generate the hydration product. This drawback could be avoided by the use of a *N*-heterocyclic carbene-gold complex. This presentation will highlight our results in this area.

Macrocyclization via dynamic kinetic resolution using a chemoenzymatic approach

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Université de Montréal

Macrolactones, or large ring esters, are common motifs found in bioactive natural products, pharmaceuticals and cosmetics. In addition to the challenges associated with macrocyclization, the synthesis of many macrolactones is complicated by installing and/maintaining the stereochemistry of the alcohol precursor. Dynamic kinetic resolution (DKR) is a powerful technique in asymmetric catalysis allowing chemists to exploit easily accessible racemic materials to prepare enantioenriched targets. Surprisingly, DKR has never been applied to any macrocyclization process. Our group has developed a chemoenzymatic approach to chiral macrolactones. Ruthenium or iron catalysts racemize secondary alcohols which can subsequently engage in a biocatalytic lipase catalyzed acylation. Optimization of the reaction conditions and exploration of the reaction scope will be presented.

Revisiting the Regioselectivity of Disubstituted Isoxazoles: Ru(II) Mechanocatalyzed Synthesis of 3,4-Isoxazoles

R. Hernandez*, P. Forgione
Concordia University

The synthesis of heterocycles has constituted a proliferating and growing area in organic chemistry. Specifically, disubstituted isoxazole motifs are among the most frequently encountered heterocycle in many drug candidates and a versatile intermediate in synthesizing natural products. Frequently, disubstituted isoxazoles are synthesized by a 1,3-dipolar cycloaddition between terminal alkynes and nitrile oxides (NOs). Under thermal conditions, the cycloaddition results in mixtures of 3,5- and 3,4-disubstituted regioisomers. Recent reports in Ru catalysis demonstrate that adding a Ru(II) complex in catalytic amounts allows the preferential formation of 3,4-disubstituted isoxazoles. However, significant drawbacks are encountered in this solution-based protocol, such as long reaction times, low atom economy, low energy efficiency, and the need for inert conditions. Alternatively, mechanochemical synthesis has been utilized in synthesizing complex organic molecules, demonstrating unprecedented modes of reactivity and selectivity with a lower environmental impact and far simple protocols. Herein, we would like to discuss the impact of the Ru(II) mechanocatalyze synthesis of 3,4-disubstituted isoxazoles from terminal alkynes and hydroxyimidoyl chlorides in short reaction times, with excellent regioselectivity and with lower waste-production than in solution-based chemistry.

Development of the thieno[3,2-c]isoquinoline scaffold as a potential anti-cancer agent

K. Mckibbon
Concordia University

Several derivatives of a series that share a thienoisoquinoline scaffold have demonstrated potent activity against cancer cell lines A549, HeLa, HCT-116, and MDA-MB-231 in the submicromolar concentration range. Structure-activity relationship (SAR) studies on a range of derivatives aided in identifying key pharmacophores in the lead compound. Ongoing SAR studies focus on more targeted modulation of the proposed pharmacophores, providing a series of compounds that have been identified as the most promising with low nanomolar IC_{50} values against patient-derived triple-negative breast cancer cells. Microscopy studies of cancer cells treated with the lead compound revealed that it causes mitotic arrest and disrupts microtubules. Further evaluation via an in vitro microtubule polymerization assay and competition studies indicate that the lead compound binds to tubulin via the colchicine site.

Synthesis of exoglycals and exoglycal derivatives as enzyme inhibitors

E. Ospanow
Dalhousie University

Carbohydrates are one of the building blocks of human life. As such they play an important role in diseases, for example cardiovascular diseases and diabetes. Interesting targets for these diseases can be enzymes, which can be inhibited by small carbohydrate-based molecules. Involved enzymes can inhibited by reversible or covalent inhibitors based on the functionalities present in the molecule. So called Exoglycals or C-glycosylidenes are carbohydrate derivatives in which the anomeric linkage is replaced by a carbon–carbon double bond. Conformationally their transition state is similar to the transition state for the enzymatic hydrolysis of the glycosidic bond, which can render them a potential inhibitor for enzymes that exhibit this transition state. As a starting point for the synthesis of exoglycals a variety of benzothiazole-based olefination reagents were prepared and used in a modified Julia olefination reaction to prepare the exoglycals as possible enzyme inhibitors.

Total and Chemoenzymatic Synthesis of Seongsanamide E

A. Paquette*, J. Brazeau-Henrie, M. Darnowski, C. Boddy
University of Ottawa

Chemoenzymatic synthesis combines the strengths of synthetic organic chemistry with the selectivity of enzymatic reactions, enabling the synthesis of challenging molecules. Thioesterases (TEs) that macrocyclize and release linear enzyme-bound substrate in the biosynthesis of macrocyclic peptides are ideal enzymes for use in chemoenzymatic synthesis since they generate synthetically challenging macrocycles in good yield and without the common side products. Herein, we report the total synthesis of seongsanamide E via TE-mediated macrocyclization of a linear intermediate. The seongsanamides are cyclic nonribosomal depsipeptides isolated from the marine sponge-associated bacterium Bacillus safensis KCTC 12796BP. Using solid phase peptide synthesis (SPPS) and solution-phase synthesis, seongsanamide E standard was synthesized via chemical macrolactamization. The N-acetylcysteamine (SNAC) derivative of the native linear sequence was generated through selective C-terminal thioesterifaction after on-resin peptide release. The excised TE from seongsanamide biosynthesis was expressed and treated with the SNAC intermediate yielding depsipeptide seongsanamide E via macrolactonization, a reaction that was not achievable using typically organic chemistry reaction conditions. The product was confirmed by comparison to our synthetic seongsanamide E standard. This study demonstrates the power of combining synthetic chemistry with biocatalysis and links the proposed biosynthetic genes with the chemoenzymatic synthesis of seongsanamide E.

Development of new antimicrobial agents based on bis-benzimidazolium salts to combat bacterial resistance

M. Petit
Université de Montréal

To address pathogenic bacteria's increasing tolerance through biofilm formation and resistance mechanisms, we thought of optimizing quaternary ammonium compounds (QAC) inspired from antimicrobial peptides. While previous studies showed their high bactericidal potential, there is still room for optimization to improve their biocompatibility and their antibiofilm properties. In this study, we rationally synthesized amphipathic biscationic quaternary ammoniums based on bis-benzimidazolium salts and investigated their biological activity, while gradually optimizing their structure. Their cationic nature allows high affinity with the anionic bacterial membrane followed by the insertion of the hydrophobic segments disrupting the membrane. Hence, bis-benzimidazolium salts displayed broad spectrum activity against Gram-positive (VRE, MRSA) and Gram-negative (E.coli) bacterial species. The biocompatibility depended on their low charge density, resulting in bis-benzimidazolium analogues which displayed less than 90% hemolytic activity against human red blood cells at high concentration. In the development of new antimicrobial, the biofilm formation and the apparition of resistance are main challenges. Owing to their fast bactericidal action, the compounds inhibited biofilm formation at low doses and an absence of increased tolerance was observed upon repeatedly exposing MRSA and E.coli to bis-benzimidazolium salts. Thus, amphiphilic cationic antimicrobials based on bis-benzimidazolium salts are promising therapeutic agents.

A Three-Pronged Approach to Design Anillin-Specific Inhibitors and Liver Cancer Treatment

S. Pilavdjian
Concordia University

Worldwide, liver cancer is the third leading cause of cancer-related deaths. Current treatment methods, such as chemotherapy, radiation and existing drugs, pose numerous patient compatibility complications. This can be avoided by targeting anillin, the protein that regulates and binds to the cytokinesis machinery. This new approach aims to overcome these limitations and parallels the new method of drug delivery enabled through structural mimetic chemistry, the field revolving around designing small molecules that mimic large regions of protein surfaces. Results obtained from molecular docking studies reveal the first generation of anillin inhibitors as 2,5-bipyridyl thiazole scaffolds containing benzyl derivatives on the central core. Conventional methods to synthesize substituted thiazole rings proceed through Hantzsch cyclization involving α-haloketones and thioamides. However, this approach requires additional steps to fabricate the starting materials and the final product suffers from the inability to undergo late-stage modification. As such, a series of palladium-catalyzed cross-coupling Suzuki–Miyaura coupling and direct C–H activation/arylation synthetic schemes were developed, allowing for tunability for a diverse variety of candidates all derived from a common building block. Future biological testing for these synthesized molecules includes the measurement of anillin inhibition *in vitro*, bimolecular fluorescence complementation and substrate efficacy in cancerous cells *in vivo*.

Repurposing Drug-Like Molecules for Applications Against Gram-Negative Bacteria through Chemical Modifications

P. Prevost
Concordia University

Antibiotic resistance presents an urgent problem, with resistant infections causing millions of deaths each year. Bacterial resistance is outpacing the development of antibiotic therapies, particularly for gram-negative bacteria, which are responsible for a variety of blood, respiratory, and food/hospital-borne infections. Gram-negative bacteria have a protective lipopolysaccharide outer membrane that reduces permeability by small molecules/drugs which must therefore enter through porins. Recent studies have determined that the molecules that best traverse porins are small rigid, amphiphilic, with low globularity and importantly, the presence of an unhindered primary amine.
Using these findings, a library of roughly 400 compounds were tested in the presence of a membrane permeabilizer against E. coli in order to find compounds that have antibiotic activity, and of the 25 positive hits found, 3 lead compounds that most adhered to the shape guidelines were selected. A total synthesis of each compound was designed that allowed for modularity as well as the presence of a primary amine. Derivatives of one lead compound were synthesized and biological testing have shown promising results, with moderate antibiotic activity against gram-negative bacteria, including strongly resistant bacteria, without the presence of membrane permeabilizers. Further derivatives are being synthesized in order to improve antibiotic activity.

Molecular Characterization of Boron Heterocycles as Biologically Active Compounds

K. Reznikov
Dalhousie University

Boron heterocycles have an impact on a variety of applications in drug discovery and medicinal chemistry. Boron-containing molecules have even been approved for drug use to treat a variety of conditions, such as multiple myeloma and lymphoma, with the boron atom critical to the drug- target interaction. In our lab, we have synthesized and investigated the properties of molecules containing a formylphenylboronic acid functionality due to the potential for iminoboronate formation with lysine residues within a target active site. An iminoboronate is a stabilized imine formed through the reversible reaction between an amino- and aldehyde functionality. The molecules were designed to interact with enzymes in the bacterial rhamnose biosynthetic pathway, a known antibiotic target. Crystallographic analysis of PDB data indicated that these enzymes contain multiple lysine residues within their active sites. Molecules were structurally comparable in volume to thymidine diphosphoglucose and thymidine diphosphorhamnose, products of the biosynthetic pathway. In this study, we have initiated the characterization of these formylphenylboronic acid derivatives to measure pKa values, imine formation constants and diol binding formation constants using a variety of UV-visible, fluorescence and NMR spectroscopic techniques. Data from these experiments will be presented and discussed.

Electrochemical Palladium-Catalyzed Carbonylation: Oxidation State Shuffling as a Catalyst Design Tool

K. M. Tam*, P.-L. Lagueux-Tremblay, M. Jiang, B. Arndtsen
McGill University

Transition metal-catalyzed carbonylation is one of the most efficient and atom-economical approaches to carbonyl-containing compounds, which are ubiquitous in nature and of great importance to pharmaceutical and material sciences. However, classical thermal reactions suffer from the need to balance properties of the metal catalyst such that distinct mechanistic steps, namely oxidative addition and reductive elimination, proceed at appreciable rates and that the catalyst is regenerated after each cycle. Herein, we describe a conceptually novel approach to catalyst design, employing electrochemical potential to drive catalysis by shuffling the oxidation states of the metal center for both product formation and catalyst regeneration. Reactive acyl chlorides are catalytically synthesized at ambient temperature and pressure, allowing for a wide array of carbonyl-containing products to be prepared from simple organic building blocks.

Optimizing alkylated ammonium-based compounds to improve ice recrystallization inhibition (IRI) and cryopreservation efficacy

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During cryopreservation, ice recrystallization, defined as the growth of larger ice crystals at the expense of smaller ice crystals, leads to non-repairable membrane damage and cell death. The development of small molecules as ice recrystallization inhibitors (IRIs) has proven to be an effective strategy to mitigate cryoinjury in various cell types. Previous work has shown that ammonium-based salts exhibit IRI activity and quaternary ammonium salts have been previously implicated as cryoprotectants. Consequently, we sought to assess various alkylated ammonium salts for IRI activity and subsequent optimization of cryoprotective properties. Preliminary studies have focused on modifications made to the quaternary ammonium salt choline chloride. Choline chloride has been shown to exhibit low cytotoxicity and is a biorelevant molecule. SAR studies on choline have yielded positive results, where modifications to the N-alkyl position(s) and the counterion yielded notable increases in IRI activity compared to the parent (IC_{50} = 20 – 40 mM vs. 235 mM). Cytotoxicity assays have demonstrated that IRI active derivatives of choline possess similar toxicity profiles to the biocompatible parent. Taken together, these results demonstrate the ability to improve the IRI activity of ammonium-based salts and highlights their potential to be used as cryo-additives in cellular systems.

MOLECULAR BIOLOGY

Biallelic variants in *TRAPPC6B* Cause Neurodevelopmental Disorder in Humans and suggest a defect in TRAPP II-specific function

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The transport protein particle (TRAPP) complexes are crucial for vesicular transport within the endomembrane system. Defects in some TRAPP subunits are associated with neurodevelopmental disorders in humans. Here we identified 7 homozygous nonsense, 7 canonical splice site mutations and a single patient with a compound heterozygous mutation with a milder phenotype. All individuals suffer from microcephalic neurodevelopmental disorder. We performed functional studies to assess the effect of the identified variants on Golgi integrity and membrane trafficking. We focused our functional studies on two individuals with the following homozygous variants: c.454C>T, p.Q152* (individuals S1 and S2) and c.149+2T>A, predicted splice variant (individuals S3 and S4). Molecular studies revealed a weakened interaction between mutant TRAPPC6B (c.454C>T, p.Q152*) and its TRAPP binding partner TRAPPC3. Patient-derived fibroblasts from S1 and S2 have reduced levels of TRAPPC6B as well as TRAPP II complex-specific members (TRAPPC2L, TRAPPC9 and TRAPPC10) Interestingly, the levels of the TRAPPC6B homologue TRAPPC6A were found to be elevated. The reduction in TRAPPC6B affects Golgi integrity and trafficking into the Golgi in both S1 and S2, as well as in S3 and S4-derived fibroblasts. Our data provide additional support for TRAPPC6B biallelic variants association with neurodevelopmental disorder and microcephaly in humans.

Novel molecular tools to increase SUMOylation of target proteins

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Protein post-translational modifications (PTMs) play a key role in cell signaling. They can, for example, modulate protein localization or their interaction with other proteins. One of these PTM, termed SUMOylation, involves the transfer of a Small Ubiquitin-like Modifier (SUMO) to a lysine residue on a protein substrate. SUMOylation is an ATP-dependant reaction which implies the sequential action of 3 proteins: an E1 activating enzyme, an E2 conjugating enzyme and an E3 ligase. SUMOylation is implicated in multiple cellular processes such as DNA repair or gene transcription. It is well established that a dysfunction of the SUMOylation reaction leads to multiple diseases such as Rett syndrome, an orphan disease affecting almost exclusively girls. While strategies have been developed to increase SUMOylation on a protein-wide level, none of them can augment SUMOylation of a specific protein. Our goal is thus to develop molecular tools to investigate the role of SUMOylation in key molecular processes and assay their usefulness for therapeutic intervention for diseases. It is thus critical to develop tools that will increase SUMOylation of a specific protein such as MeCP2, a protein whose mutation cause Rett Syndrome, to further understand the roles of SUMOylation on key proteins.

Exploiting evolution: Chloramphenicol resistance impairs evolution of resistance to antibiotics

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In Canada, approximately 15 deaths occurred every day due to antibiotic resistant infections in 2018, shrinking GDP by $2.0 billion. By the year 2050, Canada's GDP is expected to shrink by about $388 billion, and global yearly deaths caused by antibiotic resistant bacteria are expected to rise to 10 million. With a dry antibiotic development pipeline, we urgently need novel strategies to combat the evolution of resistance. Here, using high-throughput *in vitro* bacterial evolutions, I show that evolution of resistance to the antibiotic chloramphenicol severely affects bacterial fitness, slowing the rate at which they evolve resistance to other antibiotics like streptomycin and nitrofurantoin. This effect was linked to consequences of chloramphenicol resistance, as bacteria evolved against streptomycin readily acquired resistance to nitrofurantoin. *In vitro* acquisition of compensatory mutations in the chloramphenicol resistant cells markedly improved fitness, but their adaptation rates, while showing improvement against streptomycin, remained comparable to the original mutants against nitrofurantoin, indicating the impairment to be a stable, difficult-to-revert phenotype. Studies like this will be useful in identifying antibiotics that impair subsequent resistance evolution, and may help clinicians prescribe sequential antibiotic therapies that are less prone to resistance evolution.

Genetic engineering of Bacillus subtilis for usage in living functional materials

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Bacillus subtilis represents a powerful tool for recombinant expression of functional proteins. As previously shown for Escherichia coli biofilms, B. subtilis biofilms can be engineered for various applications, including tissue regeneration. As opposed to E. coli, B. subtilis does not produce lipopolysaccharides, which are proinflammatory. B. subtilis strains are generally regarded as safe, which enables their usage for the design of engineered living materials. In this study, we aim to genetically engineer B. subtilis to produce living functionalized biofilm for tissue regeneration. In this regard, we knocked out the epsA-O and the sinR and tasA genes. The epsA-O cluster is responsible for production of exopolysaccharides, which allow interaction with a hydrophobic protein covering the biofilms. SinR acts as repressor of TasA, the biofilm scaffold protein. Deletion of tasA will allow expression of functionalized biofilm via the introduction of plasmids containing tasA genetic fusions. Markerless deletions in B. subtilis were achieved by allele replacement with suicide plasmids containing flanking regions of the target genes. Deletion of the targeted

genes results in altered morphology and/or production of biofilms. Ultimately this modified strain could be further engineered for in situ production of therapeutic molecules for biomedical applications, including tissue regeneration.

Development of a Whole-Cell Biosensor for β-Lactamase Inhibitor Discovery

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The clinical utility of β-lactam antibiotics is endangered by the production of β-lactamases by multi-drug resistant bacterial pathogens, a current global health threat. Although extensive efforts have been made to develop inhibitors for these enzymes, inhibitor-resistant variants emerge rapidly. In addition, there are no clinically available inhibitors for many currently observed β -lactamases. To facilitate inhibitor discovery efforts, new assays are required to assess inhibitor efficacy in a cellular context. We describe the development of a whole-cell biosensor which can be applied to the identification of β-lactamase inhibitors, prioritizing hits that are effective against bacterial cells. Upon administration of an effective inhibitor, the co-administered β-lactam antibiotic is rescued from β-lactamase-catalyzed degradation, causing the biosensor to produce a luminescent signal. This platform was validated using a panel of clinically relevant β-lactamases and was applied to quantitatively measure the potency of currently used β-lactamase inhibitors. This assay is cost-effective and does not require the use of potentially expensive substrates. It also overcomes limitations associated with purified protein assays, accounting for inhibitor permeability and efflux, and has a significantly shorter time-to-result than the growth-based methods traditionally used for evaluating β-lactamase inhibitors.

Sheltering of B-lactam-susceptible bacterial strains by B-lactamase-producing bacteria

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B-lactams are the most used class of antibiotics worldwide. Unfortunately, their clinical utility is being threatened by B-lactamase-producing bacteria which are resistant to B-lactams. B-Lactamase production by resistant bacteria may also shelter susceptible bacterial strains, contributing to B-lactam treatment failure, particularly in poly-microbial infections. Previous studies in this area have examined sheltering using plate counting experiments. However, this is a relatively slow and low throughput approach which cannot be used to efficiently study the factors that contribute to sheltering. As such, there is a need for an easy and inexpensive method to monitor antibiotic sheltering. To address this need, we have developed a luminescent reporter system that can be used to directly monitor bacterial growth. We demonstrate that it is possible to measure sheltering with this assay, and that the level of sheltering depends on the type of B-lactamase produced and the identity of the B-lactam antibiotic used. We are currently applying this approach to characterize the factor(s) that contribute to this sheltering effect.

Evolution of Plasmid-encoded CTX-M-15 Gene Against a Set of Beta-lactam Antibiotics

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CTX-M-type extended-spectrum beta-lactamases (ESBLs) are a major driver of antibiotic resistance in Canada and the USA, conferring resistance to a broad array of beta-lactam antibiotics, including late generation cephalosporins. According to a recent study 62.3% of ESBL-containing E. coli pathogens in Canada harbour CTX-M-15, thus contributing to the spread and adaptation of high-risk clones. Considering it takes approximately ten years to develop a new antibiotic, and only three days for bacteria to develop resistance, we must understand how CTX-M-15 will mutate in the coming years.
In this talk I will present my work on the evolution of CTX-M-15 in soft agar. Using the soft agar gradient evolution (SAGE) technique antibiotic resistance can be evolved in 4-7 days. Evolution is currently being directed against two types of beta-lactams: (i) those currently prescribed for the treatment of ESBL-related infections like carbapenems and (ii) those towards which the ESBL pathogens have previously evolved high resistance like cefotaxime. Sequencing of evolved genes will provide insight into how resistance evolves, while inhibitory tests probe for cross-resistance and collateral sensitivity. Overall, this work will help identify treatment regimens that may delay the evolution of antibiotic resistance genes in the clinic.

BIOCHEMISTRY

Development and optimization of mechanoenzymatic plastic depolymerization: a novel approach to plastic recycling

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Plastic is essential to our daily lives, and as a result, we produce millions of tons of plastic every year. Unfortunately, only a very small fraction of plastic is recycled, and the recycling processes available are not efficient. The use of enzymes as natural catalysts for plastic degradation presents an exciting opportunity for an environment-friendly recycling that can break plastics down to their monomers, while avoiding the use of harsh chemicals or conditions. Recently, our group developed a novel technology that uses enzymes in mechanically mixed, moist-solid reaction conditions, which requires only a few equivalents of water. While dramatically different from the traditional dilute, aqueous, enzymatic reaction conditions, this technology has proven efficient for the depolymerization of natural polymers such as cellulose, hemicellulose, and chitin, as well as synthetic polymers including polyethylene terephthalate, polylactic acid, and polyester textiles. With the goal of expanding upon this technology and applying it more widely to other plastics, my talk will focus on my recent work towards the depolymerization of nylon-6,6 and

poly-(3)-hydroxybutyrate. Overall, this work represents an important step towards achieving a circular plastics economy, and therefore an important step in tackling the plastic pollution problem.

Screening Indigo Formation for Predicting Substrate Promiscuity in Cytochrome P450 BM3 Libraries

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Biocatalytic routes for chemically challenging syntheses have been developed recently. Among these, cytochrome P450 oxidases (P450s) promote oxidation reactions. The P450 from Bacillus megaterium (P450 BM3) natively hydroxylates terminal, non-activated C-H bonds of long-chain fatty acids. P450 BM3 has been engineered for the hydroxylation of short-chain fatty acids, aromatic compounds, terpenes and alkanes. Given the potency of P450s for chemical synthesis, a substrate promiscuity study on large-scale P450 libraries is required using efficient high-throughput screening methods. Colorimetric high-throughput, whole-cell screening to observe the conversion of indole to indigo has identified a correlation with increased substrate promiscuity in a small number of P450 variants. We explored the conformational space of P450 BM3 and characterized 78 new indigo-producing variants and 53 non-indigo-producing variants for promiscuous aromatic hydroxylation. 70-80% of indigo-producing variants performed better than WT for oxidation of anisole and naphthalene, compared to 40-45% of non-indigo-producing variants. All top variants (3-fold or more activity increase over WT) were indigo producers. Overall, cost-effective and sensitive screening by colony-based colorimetric observation has allowed selection of point-mutated, indigo-producing P450 BM3 variants displaying improved aromatic oxidation. The top selected promiscuous variants and the diversity of substrate classes that correlates with indigo formation will be further investigated.

Synthesis of a fluorogenic photocrosslinker probe to capture glycan-protein interactions

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Sugars are central elements in biology as complex glycans participate in various physiological and pathological processes. For example, recognition of glycans by glycan-binding proteins known as lectins is often key to cellular communication, to cell adhesion and to pathological processes in the case of cancer cells presenting perturbed glycosylation. A significant challenge in the field is to capture and visualize these sugar-protein interactions, in part because of their usually low affinity. Photocrosslinking is often used to capture interacting biomolecules. When activation with light can induce reactive intermediates such as carbenes and nitrenes, crosslinker probes can insert in molecules in close proximity and create covalent bonds. However, certain photoreactive motifs such as aryl azides have proven prone to non-productive rearrangement. Fluorination of the aromatic core is an attractive solution to improve nitrene reactivity preferentially towards insertion in proximal bonds. Additionally, azides appended on chromophores are known to quench their fluorescence. In this work, we developed a fluorogenic photocrosslinker by combining stabilizing effects of fluorine atoms and quenching properties of the azide on a coumarin scaffold. Attaching this new probe to an α-fucose sugar, we demonstrate the proof-of-concept for fluorogenic capture of glycan-protein interactions using two fucose-binding lectin models.

AlphaFold predicts functional protein-protein interaction

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Proteins are molecular machines that control every biological process in cells. Proteins are dynamic, and the interactions between them coordinate their mobility and, consequently, their cellular function. AlphaFold, an artificial intelligence system developed by DeepMind, has the potential to revolutionize our understanding of biology. Successfully, our team demonstrates that AlphaFold's predictive power can be harnessed to elucidate novel protein-protein interactions of RNF13, a transmembrane ubiquitin E3 ligase involved in multiple pathological dysfunctions. Of particular interest to us was the dileucine motif of RNF13 that is altered by the L311S and L312P variants causing the developmental and epileptic encephalopathy 73. Here, we used AlphaFold to distinguish real interactors from proteins only found in the vicinity of the bait. For our first analyses, we used BioGrid where multiple RNF13 interactors have been reported, mostly from high throughput mass spectrometry assays. Whereas Alphafold failed to predict the binding of CLCN7 with RNF13 as reported in BioGrid, Alphafold clearly predicted that the clathrin adaptor proteins AP-1 and AP-3 binds the dileucine motif of RNF13, and allowed us to direct our experiments regarding RNF13's pathologic variants L311S and L312P. Our study will also present other interactors of RNF13 that have been validated using biochemical assays.

Cofactor-Free Continuous Flow Biocatalysis System for Potential Low-Cost Applications Using the Cytochrome P450 Enzyme

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Variants of the enzyme cytochrome P450 oxidase have been engineered by laboratory evolution for increased production of indigo (an industrial dye) and raspberry ketone (a flavor in high demand in the food industry). To make these enzymes industrially attractive, optimization of the production yield and reduced cost are necessary. In this work, we replaced the NADPH cofactor of the enzyme cytochrome P450, which is excessively expensive in the context of industrial production, with mediated electron transfer. It is based on a sacrificial electron donor and a photoactivated electron transfer mediator that transfer electrons to the active site to promote the oxidation reaction. The biocatalytic reaction was performed in a transparent flow reactor for activation

of electron transfer by visible light. The cytochrome P450 BM3 enzyme was purified and immobilized in one step on Ni-NTA activated resin, inside the reactor. Several combinations of electron donor and electron transfer mediator (eosin Y and rose Bengal) were investigated to perform the biocatalytic reaction in optimal conditions and prevent enzyme inactivation. Reaction parameters such as reactor volume, light intensity and reaction time were investigated to optimize the yield. Enzyme stability toward continuous catalysis and storage conditions were also investigated, to optimize the catalytic efficiency.

Non-SELEX method for Aptamers Selection to H3 domain peptide of SARS-COV-2 Envelope protein

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The genomes of all corona-viruses encode four major structural proteins: the spike (S) protein, the nucleocapsid (N) protein, the membrane (M) protein, and the envelope (E) protein. The E protein is possibly the most interesting of them since it is associated with the promotion of virus-host interaction and pathogenesis. In order to better target virus in human body, the protein on the surface of virus is always been selected as biomarker. The H3 peptide is the only domain that exposes on the surface of SARS-COV-2, so it is more promising if the aptamer that can selectively bind with H3 peptide is selected. As for an aptamer, it is a highly specific DNA ligand, raised to identify virtually any target molecule through an iterative process known as SELEX (systematic evolution of ligands by exponential amplification). Our focus is using non-SELEX selection of aptamers, a process that devoid of any aptamer amplification during the selection process. Thus shorten the time and the efficiency has been raised. By carrying out all of the studies, the results have potential to be helpful in development of anti-SARS-CoV-2 medications, and for understanding the function of viroporins in general.

Exploring the effects of substrate post-translational modification on the structural dynamics of a lanthipeptide synthetase

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Lanthipeptides belong to the family of ribosomally synthesized and post translationally modified peptide (RiPP) natural products. Lanthipeptides are genetically encoded precursor peptides that undergo multistep modification catalyzed by lanthipeptide synthetases. These enzymes function iteratively during the stepwise modification of the precursor peptide into a structurally complex peptide macrocycle, which often exhibits antibiotic activity. The relaxed substrate specificity of lanthipeptide (and other RiPP) synthetases likely results, in part, from conformational changes of lanthipeptide synthases in presence of their substrate(s). In this study, we have utilized hydrogen-deuterium exchange (HDX) and Native Mass spectrometry to investigate the effects of substrate post-translational modification on the conformational changes in the model class II lanthipeptide synthetase, HalM2. Consistent with our hypothesis, we found that post-translational modification can affect the global and local dynamics of HalM2. For some regions of HalM2, the HDX perturbations can be related specifically to HalA2 stepwise modification. The data further illustrate the power of structural mass spectrometry for illuminating interactions in biosynthesis pathways.

Pantothenamide-Mimicking Compounds: A New Class of Antimicrobial Agents

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Antimicrobial resistance is rapidly increasing each year, posing a significant menace to modern medicine. In 2019, antimicrobial resistance joined air pollution and climate change in the World Health Organization's top ten global public health threats facing humanity. Pantothenamides are a new class of antimicrobial agents that exhibit a new (and often multiple) mechanism(s) of action, making them alluring new agents in the battle against antimicrobial resistance. They act by utilizing bacterial and parasitic coenzyme A enzymes that bioactivate pantothenamides into corresponding coenzyme A antimetabolites that can infiltrate further downstream coenzyme A utilizing processes, resulting in bacterial/parasitic cell death. However, due to pantothenamides' susceptibility to cleavage by enzymes called pantetheinases in human serum, synthetic techniques have been employed to limit pantetheinase-related degradation. This talk will discuss the synthesis and biological testing of novel pantothenamide-mimicking compounds.

Structural polymorphism of guanine quadruplex-containing regions in human promoters

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Intramolecular guanine quadruplexes (G4s) are non-canonical nucleic acid structures formed by four guanine (G)-rich tracts that assemble into a core of stacked planar tetrads. G4-forming DNA sequences are enriched in gene promoters and are implicated in the control of gene expression. Most G4-forming DNA contains more G residues than can simultaneously be incorporated into the core resulting in a variety of different possible G4 structures. While this kind of structural polymorphism is well recognized in the literature, there remain unanswered questions regarding possible connections between G4 polymorphism and biological function. Here we report a detailed bioinformatic survey of G4 polymorphism in human gene promoter regions. Our analysis is based on identifying G4-containing regions (G4CRs), which we define as stretches of DNA in which every residue can form part of a G4. We found that G4CRs with higher degrees of polymorphism are more tightly clustered near transcription sites and tend to contain G4s with shorter loops and bulges. Furthermore, we found that G4CRs with well-characterized biological function tended to be longer and more polymorphic than genome-wide averages. These results represent new evidence linking G4 polymorphism to biological function and provide new criteria for identifying biologically relevant G4-forming regions from genomic data.

A Scalable Hemoglobin Bis-Tetramer Synthesis for Use Towards Pre-Clinical Studies

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Pre-clinical mice studies of bis-tetramers, a type of hemoglobin-based oxygen carrier(HBOC), have demonstrated that they overcome all adversities associated with previous generation HBOCs. The current bis-tetramer synthesis, however, struggles with scalability, largely due to an unreactive side-product that cannot undergo a critical protein-protein conjugation step. This side-product contains a cross-link between the a-subunits of hemoglobin(Hb), while the desired product is cross-linked between the b-subunits. The formation of this unreactive a-cross-linked by-product significantly restricts yields and serves as a bottleneck towards scaling up the bis-tetramer protocol. We find that by cross-linking Hb in the R-state, the undesired reactions at the a-subunits are prevented. Although the target b-subunit site is most accessible in the T-state conformation, where Hb is normally cross-linked, the undesired a-site is also accessible, causing side reactions. Contrarily, in R-state Hb the b-site is only relatively hindered while the a-site is very hindered. Reacting R-state Hb, however, caused reduced yields at the target b-site. We find that by minimizing steric bulk on the cross-linker, its reactivity towards the R-state b-site increases, affording high yields. Optimizing the bis-tetramer synthesis by the combined use of R-state Hb and the modified cross-linker ultimately produced a scalable synthesis for further pre-clinical studies.

Mapping Concussion for Early Diagnosis by Molecular MRI

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Concussion is a form of mild traumatic brain injury (mTBI), defined as complex neurological impairment induced by biomechanical forces without structural brain damage, and is invisible to standard imaging. The lack of objective diagnostic tools for concussion has identified a need for molecular imaging probes targeted to the diagnosis of mTBI. Downstream injury from mTBI stems from oxidative damage, leading to the production of neurotoxic aldehydes. A novel CEST-MRI contrast agent, 5-propargyloxy-2-hydrazinobenzoic acid (PHBA), has been developed to map aldehyde production in vivo following mTBI. PHBA binds rapidly and irreversibly with aldehydes, affording the use of pathology-associated aldehydes as imaging biomarkers for MRI. A mouse model of closed-head, awake concussion was developed in a strain of aldehyde dehydrogenase 2 knockout mice. CEST-MRI was performed on days 2 and 7 after impact. Signal enhancement significantly increases at 2 days post-injury and returns to baseline by 7 days in all mice. This novel MRI contrast agent represents the first objective diagnostic tool for concussion using aldehydes as a biomarker for injury. These probes may eventually be used in a clinical setting to accurately diagnose concussion and map the location and severity of injury.

Identification of new nucleolar HBZ-associated proteins in chronically HTLV-1-infected cells

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Adult T-cell leukemia/lymphoma (ATL), an aggressive CD4+ T-cell malignancy, develops in 2–5% of individuals chronically infected with human T-cell lymphotropic virus type 1 (HTLV-1). HTLV-1 basic Zip factor (HBZ) is a viral protein, which plays a crucial role in developing ATL. Based on our previous results and hypothesis that its nucleolar localisation is determinant for its transformation-inducing properties, a reliable method for extracting nucleoli from different cell lines was developed. Nucleolar localization of HBZ was first confirmed by western blot and confocal microscopy. Using co-immunoprecipitation and confocal microscopy on transiently expressing HEK293T as well as chronically infected non-T and T cell lines, we further showed that this protein was associated to NPM1/B23 protein, a nucleolar component that plays a variety of roles, including ribosome biogenesis. We are currently optimizing a proximity-dependent biotinylation (BioID2) approach to identify additional nucleolar proteins associated to HBZ. Altogether, our result suggests that nucleolar localization of HBZ leads to specific association to interacting partners contributing to its implication in ATL development.

A Series of Controlled Movements Mediate Enzyme Activity: Conformational Dynamics in Cytochrome P450 Reductase

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Cytochrome P450 enzymes (CYPs) and their redox partner, cytochrome P450 reductase (CPR), play important roles in the metabolism of small molecule medicines. CPR is a reductase that mediates electron transfer from nicotinamide adenine dinucleotide phosphate (NADPH) to the heme prosthetic group of CYPs via two tightly bound flavin co-factors. Proper heme reduction is required for CYP function, making CPR activity absolutely essential. The past few decades have led to major advances towards understanding the mechanistic features of CYPs; however, less attention has been given to CPR. Currently, it is known that CPR reduction involves structural changes that alter CPR activity and influence its interactions with CYPs. Moreover, mutations that negatively impact CPR function are thought to have serious consequences on human health. It is suspected that many of these clinically relevant mutations affect CPR function by altering CPR structural dynamics. However, we must first develop a concrete understanding of the dynamics of the wild type enzyme. Our lab uses a technique called hydrogen-deuterium exchange mass spectrometry (HDX-MS) to study local changes in enzyme structure. Using HDX-MS, we are working towards developing a fundamental understanding of the dynamics involved in CPR function. This presentation will summarize our most recent findings.

The bacterial itaconate degradation pathway: an immune system evasion mechanism and antimicrobial target

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In the fight against antimicrobial resistance, it is crucial that we not only develop new antibiotics but also alternative treatments with a reduced frequency of resistance development. The Auclair group has pioneered a new strategy to resensitize intracellular bacteria to our immune systems which consists of inhibiting bacterial itaconate degradation. During an infection, macrophages engulf bacteria and kill them through a variety of mechanisms, including the use of antimicrobial molecules. Itaconate is one such molecule that blocks a metabolic pathway required for bacterial survival within macrophages, thus selectively killing them. Some pathogens such as Salmonella enterica ser. Typhimurium, Pseudomonas aeruginosa and Mycobacterium tuberculosis have evolved to express itaconate-degrading enzymes that help them to survive intracellularly. This three-enzyme pathway converts itaconate into molecules that can be used as a carbon source for bacteria. Our project aims at demonstrating that inhibition of the itaconate degradation pathway is a promising approach for the treatment of infections. To achieve this goal, we use in vitro assays at the enzyme and cellular levels, while designing inhibitors using a prodrug strategy where molecules are selectively activated by the bacterium's coenzyme A biosynthetic machinery. This presentation will summarize our progress with studying and inhibiting bacterial itaconate degradation.

Schizosaccharomyces pombe tRNA nucleotidyltransferases: A tale of two genes

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Transfer RNA nucleotidyltransferases (tRNA-NTs) have provided insights into the catalytic activity and evolution of nucleic acid modification enzymes. As tRNA-NTs ensure that tRNAs contain a 3'-cytidine-cytidine-adenosine (CCA) terminus for amino acid attachment, they are essential enzymes in eukaryotes. My research focuses on *Schizosaccharomyces pombe*, the first eukaryote shown to possess tRNA-NTs with separate CC- (*cca1*) and A- (*cca2*) adding activities. To explore why *S. pombe* has separate activities when most eukaryotes have a single CCA-adding enzyme, we showed that the *Saccharomyces cerevisiae* CCA-adding activity was sufficient to complement the loss of either or both *S. pombe* enzymes showing that neither enzyme alone possessed additional activities that were required for *S. pombe* viability. We also used a combination of two-hybrid and proximity-labelling approaches to search for interactions between the two tRNA-NTs and other proteins responsible for their activity and localization. We found aminoacyl tRNA-synthetases in proximity to both enzymes and a nuclear pore component close to *cca*1. Our data suggest that while neither protein has ancillary functions, the separate gene products may be targeted through different processes within *S. pombe*. These findings highlight the complexity of CCA addition and continue to expand our knowledge of the diversity of tRNA-NTs.

Live-cell imaging reveals impaired detoxification of lipid-derived electrophiles is a hallmark of ferroptosis

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Ferroptosis is a recently described cell death pathway characterized by iron-dependent lipid peroxidation and lipid hydroperoxide accumulation. Despite the emergence of ferroptosis as a key target of both cancer and neurodegenerative disease research, the mechanism linking lipid damage with cell death has remained elusive. We investigated lipid-derived electrophiles (LDEs) as a potential mediator of ferroptotic cell death, as the formation of LDEs through lipid hydroperoxide breakdown is known to cause cellular damage through membrane permeabilization and protein denaturation. Applying fluorescence microscopy with a fluorogenic (turn-on) LDE mimic, we studied, in real time, LDE accumulation and detoxification in cells undergoing ferroptosis. With this strategy, we not only discovered LDE detoxification impairment as a novel hallmark of ferroptosis, but also identified failure of cellular LDE detoxification as a critical stage of ferroptotic cell death.

Investigating Lipid Peroxidation Cell Death via a Fluorogenic Tocopherol Analogue Probe

W. Zhang*, G. Cosa
McGill University

Ferroptosis is a form of non-apoptotic, regulated cell death associated with lipid hydroperoxide accumulation. Ferroptosis provides a possible therapeutic opportunity in the treatment of cancers and neurodegenerative diseases. Key to understanding the molecular and cellular mechanism behind the lipid oxidative processes in ferroptosis is the monitoring of when and where lipid peroxidation occurs. Utilizing a fluorogenic probe of lipid peroxidation, here we illustrate cutting-edge live-cell fluorescence imaging studies on the progression and course of ferroptosis in real time. Our work provides both the spatiotemporal relationships of lipid peroxidation and ferroptosis, as well as its quantification.

Small Molecule Growth Inhibitors from *Onnia tomentosa* Native to British Columbia

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British Columbia (BC) is Canada's second-largest home for mushrooms, given its unusual geological history and wide climatic variations. Literature studies on *Onnia tomentosa* showed that no bioactive compounds had been isolated, nor has any bioactivity been described from this species. Bioactivity-guided fractionation and purification of *O. tomentosa* ethanol extract followed by HPLC-MS/MS and 1D/2D NMR analyses led to the identification of eight known linoleic oxygenated fatty acids (1.1-1.4, 2-5)

together with linoleic acid (**6**) and oleic acid (**7**) in the active fractions. Compound **5** was reported for the first time as the autoxidation product of linoleic acid. Subsequent GC-FID analysis was used to quantify the major fatty acids found in *O. tomentosa* together with three other selected mushrooms, including *Fomitopsis officinalis*, *Echinodontium tinctorium*, and *Albatrellus flettii*. Linoleic (15.9- 51.7 %), oleic (22.8- 57.1 %), palmitic (6.0- 14.6%), and stearic (3.7- 10.4) acids were determined as the major fatty acids in the four studied mushroom species and were reported for the first time. The cytotoxicity MTT assay indicated that linoleic acid, oleic acid, and linoleic acid autooxidation product mixture displayed antiproliferative activity against HeLa human cervical cancer cells.

ENVIRONMENTAL CHEMISTRY

Lignin-derived heterogeneous catalyst for biodiesel synthesis

A. Hamilton
Concordia University

Biodiesel has emerged as a promising alternative energy source for fossil fuels due to its renewability, biodegradability, and increased sustainability. However, current biodiesel production uses refined vegetable oils as feedstock which has raised concerns due to the competition with food crops and contributes a staggering 90% to the overall cost of production. Additionally, a major hurdle in the sustainability of biodiesel production is the current basic homogeneous catalysts employed often contaminate the product and require purification steps, resulting in substantial wastewater. For this reason, acidic heterogeneous catalysts have garnered interest as more suitable alternatives. As well as being able to perform the transesterification of triglycerides, acidic catalysts also catalyse the esterification of free fatty acids present in most non-edible and waste cooking oils into biodiesel. In this study, a lignin-derived heterogeneous catalyst converted over 97% of oleic acid- a representative of free fatty acids- into biodiesel. Furthermore, to account for the triglycerides in waste-cooking oil, a lignin-derived basic heterogeneous catalyst was also synthesised and converted over 97% of canola oil- a representation of triglycerides- into biodiesel. The replacement of homogeneous catalysts with heterogeneous offers reusability, increasing the sustainability of the biodiesel process, encouraging its adoption on a global scale.

Monitoring of select tire-derived organic chemicals in urban air

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Tire-contamination has received growing environmental concern due to its wide presence in the urban environment and potential for toxicity. However, investigations of the chemical constituents of tire pollution have mainly been limited to metals and a few common organic chemicals. Consequently, there remained a need to investigate other organic tire constituents in urban air. A literature review was conducted to identify likely tire contaminants and a suspect list including various cyclic amines, benzotriazoles, benzothiazoles, and p-phenylenediamine compounds was compiled. To obtain a global dataset for these tire-derived contaminants, archived air samples from global megacities were screened. Of the analyzed contaminants, diphenylguanidine was the most frequently detected across the globe. Other tire-compounds, such as 6PPD-quinone and benzothiazole, were also commonly detected. Although these chemicals have been associated with tire-wear, there remains a need to investigate the utility of these compounds as markers for tires as many of them have other anthropogenic sources. As a result, samples from various source sections were screened for the presence of tire-derived contamination. Diphenylguanidine and 6PPD-quinone concentrations were primarily associated with road traffic, highlighting their potential as tire-pollution indicator compounds. This study presents some of the first data for airborne concentrations of chemicals associated with tires.

A Kinetic Study on the Degradation and Biochemical Fractionation of Organic Matter in the Biggest Semi-Enclosed Estuary System of the World: an Isotopic and Genomic Approach

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Preserving the health of estuarine ecosystems has been an increasing challenge in the recent past with the spreading of areas affected by deep-water hypoxic conditions. Hence, it is of critical importance to identify the causes of such perturbation. Estuaries are large deposition centers for organic matter (OM) where stable carbon isotope ratios of either bulk OM or specific organic compounds provide detailed information about carbon cycling and the tracing of OM sources and transformations along the terrestrial-marine continuum. In particular, the $\partial^{13}C$ values of biomarkers that are specific to heterotrophic bacteria (branched iso- and anteiso-C15:0 fatty acids) can be used to assess the type of OM that they preferentially degrade as the $\partial^{13}C$ values of marine organic carbon (OC) are more enriched in ^{13}C than those of terrestrial OC. However, very little is known on the dynamics between the seasonally varying relative inputs of terrestrial vs. marine OM and the $\partial^{13}C$ values of these bacteria-specific fatty acids. In this study, we will use a kinetic batch incubation approach in which natural sediments from the St. Lawrence Estuary and Gulf, amended with fresh terrestrial or marine OM characterized by a very different $^{13}C/^{12}C$ ratio.

Non-targeted screening of organic compounds of potential concerns in urban aquatic environment

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The urban region is a reservoir of a large number of organic chemicals, many of which can enter aquatic environment via pathways such as snow melting, storm water runoff, and wastewater discharge. Environmental monitoring for organic chemicals along these pathways is limited to only a small set of chemicals. With the objective of finding lesser-known chemicals that can cause aquatic risk, we sampled snow and surface water influenced by various sources of chemicals. Methods were developed for sample preparation based on solid-phase extraction and instrumental analysis using an Orbitrap high-resolution mass spectrometer. Based on the full-spectra data, we applied non-targeted screening approaches using Compound Discoverer to investigate distributions of all the detected chemical features. Multivariate statistics were used to filter chemicals with source contributions from municipal wastewater effluent, roadway runoffs, and dry weather storm water drains. These compounds were tentatively identified based on their MS2 spectra and search of databases. Some of the compounds are potential transformation products of industrial chemicals. We report semi-quantitative abundance of the chemicals in the water samples based on the area of detected chromatographic peaks and quantitative measurements for selected compounds. The preliminary results will serve as references for planning of larger scale monitoring campaign.

COMPUTATIONAL CHEMISTRY

Searching for repurposed inhibitors of ricin through molecular modeling techniques

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Castor oil is an important product for the industry as well as the economy of several countries. However, it is also the source of ricin toxin, a chemical weapon with no known antidote. In order to identify repurposed antidotes against ricin, we have built, using different databases, a library of 82 compounds selected by virtual screening (VS) followed by docking studies. These compounds are potential binders of both the catalytic and secondary pockets of the ricin chain A (RTA). Here we report additional molecular modeling studies on a group of 15 compounds selected from this library. Steps of flexible docking followed by molecular dynamics (MD) simulations enabled to elucidate the fingerprints of these compounds inside RTA besides updating the list of the most important residues for the ligand binding. Finally, additional MM-PBSA (Molecular Mechanics Poisson–Boltzmann Surface Area) calculations allowed ranking these compounds, as well as elucidating their dynamic behaviors inside the RTA, besides pointing to the 4 most promising compounds as potent RTA inhibitors.

VIRTUAL CHEMIST or computer-aided design in asymmetric catalysis

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The field of asymmetric catalysis has revolutionized organic synthesis over the past fifty years, not only by making new reactions possible or faster, but also by promoting the synthesis of a single stereoisomer as the main product. However, the development of new chiral catalysts remains a real challenge that often results in a long and laborious process, requiring the synthesis and evaluation of several ligands and catalysts in an iterative manner. Over the past decades, virtual screening has been widely adopted as a molecular design tool in medicinal chemistry to accelerate drug discovery. In contrast, computational chemistry remains underutilized as a method for catalyst prediction and design. In order to assist the discovery of new catalysts, we propose the integration of synthetic organic chemistry and computational chemistry. We then developed ACE, a unique enantioselectivity prediction program for asymmetric reactions coupled with a fully automated software platform, VIRTUAL CHEMIST. We then succeeded in reproducing more than 350 experimental enantioselectivities for seven classes of reactions with a low enough error to distinguish the classes of stereoselectivities and determine the main product obtained in a reaction. We will present the latest progress of the project and its applications.

Structure, Dynamics, and Oligomerization of Host Defense Peptides: Elucidating the Effect of Charge, Hydrophobicity, and Chirality Using Atomistic Biomolecular Simulations

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Truncated host-defense peptide derived from mini-chicken Angiogenin 4 (mCA-4, CRFKFRIVIC) is a membrane active peptide displaying antibacterial properties. The sequence of mCA-4 can significantly affect its structure and function: (i) changing the hydrophobicity and charge of mCA-4 via amino acid substitution can modify its antibacterial efficacy; (ii) mCA-4 in a cyclic conformation is more structurally stable compared to its linear analog. The ability to change the structural and functional properties by minor sequence perturbations make mCA-4 a promising candidate for antibiotic research. This work focuses on elucidating the effect of charge, hydrophobicity, and chirality on the structure and dynamics of single and multi-chain mCA-4 systems. To investigate the effect of hydrophobicity on the structure, we study the native mCA-4 (cyclo(CRFKFRIVIC)) and a valine substituted analog (cyclo(CRFKFRVVVC)) as well as their linear analogues. To study the effect of chirality, we compare the L and D configurations of the peptides. Our results show that the native peptide is more structurally flexible and interconverts between alpha helical and beta-sheet conformations; and the valine substitution stabilizes the beta-sheet conformation. Ongoing analysis will identify: (i) the effect of chirality on peptide structure; and (ii) the mechanism of oligomerization.

Interaction Between Antimicrobial Peptide Magainin 2 and Non-lipid Components in the Bacterial Outer Envelope

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Antimicrobial peptides (AMPs) offer advantages over conventional antibiotics; for example, bacteria develop more resistance to small-molecule antibiotics than to AMPs. The interaction of the AMPs with the lipopolysaccharide (LPS) layer of the gram-negative bacteria cell envelope is not well understood. A MARTINI model was constructed of a gram-negative bacterial outer membrane interacting with the AMP Magainin 2. In a 20 μs molecular dynamics (MD) simulation, the AMP diffused to the LPS layer of the cell envelope and remained there, suggesting interactions between the Magainin 2 and the LPS layer, causing the AMP to concentrate at that position. The free energy profile for the insertion of the Magainin 2 into the membrane was also calculated using umbrella sampling, which showed that the AMP positioned such that the cationic side chains of the AMP coordinated to the negatively charged phosphate groups of the LPS layer. These simulations indicate that the AMP Magainin 2 partition into the LPS layer of a bacterial membrane.

High-throughput screening and DFT characterization of bimetallic alloy catalysts for the nitrogen reduction reaction

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The production of ammonia through the environmentally friendly electrochemical nitrogen reduction reaction (NRR) faces two major challenges, low catalytic activity, and low Faradaic efficiency, which result from poor nitrogen (N2) adsorption and the competing hydrogen evolution reaction. The d-band model offers a simple, yet effective, means to evaluate the activity and selectivity of a transition metal surface, and alloying has been found to be a suitable approach to tune the d-band of transition metals in these catalysts. However, determining the optimized composition and structure of alloys for catalysis is experimentally and even computationally very demanding. Machine learning algorithms are accurate and effective tools for screening purposes, and they are used for preliminary screening of bimetallic alloy surfaces with different stoichiometric ratios. The d-band features of various metal surfaces available from density-functional theory (DFT) datasets along with the intrinsic characteristics of the adsorption sites are used as surface descriptors. The most promising alloys are further investigated through DFT characterization of the reaction free energy profiles in order to determine the potential limiting step of NRR, assess the feasibility of the reaction by predicting the theoretical overpotential, and guide companion experimental investigations.

MLXDM: Extends Neural Network Potential to Describe Long-range Dispersion Interaction

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High-dimensional neural network potential (HDNNP) is a new computational tool that can achieve accuracy on par with high-level ab initio methods at a computational cost comparable to molecular mechanical models. Due to the short cut-off radius, HDNNP can only describe short-range interaction and lacks essential long-range interactions like electrostatics and dispersion. This research presents MLXDM, a machine learning model to predict the dispersion energy following the exchange-hole dipole moment (XDM) model. Instead of predicting dispersion energy directly, MLXDM uses artificial neural networks to predict coefficients of the XDM model, hence capable of describing interactions at an arbitrary distance. The model shows high agreement with conventional density-functional theory (DFT) dispersion corrections, with a regression coefficient (R2) of 0.975 and the mean absolute error (MAE) of 0.051 kcal/mol. To create a ready-to-use ML energy for molecular simulation, we combine the model with TorchANIPBE0, a similar HDNNP to TorchANI with the PBE0/aug-cc-pVTZ method as the reference energy. We show that the method can be used in molecular dynamics to improve the results and gain inside knowledge of the system.

NANOCHEMISTRY

Highly NIR-II Scattering Gold Superclusters for Optical Coherence Tomographic Molecular Imaging

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Near-infrared II (900 – 1700 nm, NIR-II) imaging is important in biological systems, with high tissue penetration due to limited light attenuation. Biocompatible nanomaterials capable of NIR-II imaging would enable novel investigations of biomolecular changes in living subjects. These materials would particularly impact optical coherence tomography (OCT), which is the main clinical tool used for identifying atherosclerotic plaques and placing/evaluating arterial stents. OCT is, however, limited to anatomical imaging only due to a lack of purpose-engineered contrast agents.Our work has redesigned the synthesis of metal superclusters of various plasmonic metals, as well as having led to the development of a novel AuSC with optimal OCT contrast agent properties. We have characterized a system that relies on the hydrophobic coating of precursor NPs driven to aggregation by the amphiphilicity of the stabilizing polymer-containing solvent in order to lock clusters into the desired shape. This method has led to the formation of our novel AuSCs of ~420 nm diameter with a large NIR-II LSPR peak (~1350 nm), as well as excellent aqueous dispersibility, making them well-suited to OCT molecular imaging. Our AuSCs also show a 2.5-fold greater increase in OCT signal intensity compared to regular 500 nm AuNPs.

Phospholipid bilayers as a platform for photoactivated delivery of antimicrobial peptides

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In this work, we explore the use of biocompatible phospholipid bilayers as a platform from which to deliver the antimicrobial peptide GL13K. The model is designed such that the bilayer will have an exposed alkyne group. The antimicrobial peptide GL13K was synthesized with both an o-nitrobenzyl photolabile group and an azide moiety selectively added to the central lysine residue. This enables the peptide to be tethered to the phospholipid bilayer using a copper(I)-catalyzed azide-alkene cycloaddition click reaction. In this presentation, two applications of the model will be discussed: an antimicrobial liposome formulation and the tethering of the peptide to upconverting lanthanide-doped nanoparticles (LnUCNPs) via a photocleavable linker. LnUCNPs are excited by near-IR light, which avoids potential skin damage and increases the depth of penetration of the light. These nanoparticles have the ability to absorb multiple photons and release higher energy light in the visible or UV regions. A supported lipid bilayer at the surface of the nanoparticle confers biocompatibility. Characterisation, tethering and release of the peptide, size, and stability of both liposomes and supported lipid bilayer coated nanoparticles will be demonstrated using dynamic light scattering, circular dichroism, MS and ATR-FTIR. Future applications for treatment of bacterial infections will be discussed.

Exploring Manganese (II) Doped CdS Quantum Dots for Enhanced Photoredox catalysis

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Photoredox catalysis is a continuously expanding field that seeks new, green synthetic routes to molecules of interest. Current research focuses on transition metal complexes. These metals have high costs, low availability, and rigid redox potentials. Colloidal nanocrystal quantum dots (QDs) are a new class of materials that rival precious metal complexes. QDs are stable, low-cost, and versatile. They have tunable bandgaps and long lived excited states. This makes them desirable for consumer display technologies, biological imaging techniques, and light harvesting applications such as photoredox catalysis. We investigate manganese (II) doped CdS (Mn:CdS) for photoredox reactions. The Mn (II) dopant in CdS produces a long-lived excited state, which has been shown to enhance Auger process that gives rise to hot electrons. We compare the performance of doped QDs vs undoped QDs in model photoreduction reactions where thin films of QDs were applied as heterogeneous catalysts. We observed greater than 2-fold increase in the photoreduction of an electron acceptor by Mn:CdS than CdS. A model dehalogenation reaction via photoexcitation of Mn:CdS catalyst was examined. Preliminary results suggest that an increased number of the “hot” electrons can enhance the process and allow the reaction to proceed under mild conditions.

The effect of host material on lanthanide-doped radioluminescent nanoparticles

S. L. Maurizio*, G. A. Mandl, M. D. Long, J. A. Capobianco
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Radioluminescent and scintillating materials have complex mechanisms that govern their luminescence, leaving many uncertainties in their understanding. This is further complicated when studying nanoscale materials, where the incident ionizing radiation can interact with the surrounding medium, such as surface ligands, solvent molecules, or even multiple nanoparticles. Therefore, radioluminescence research at the bulk scale may not carry over to nanoscale materials, and needs to be investigated independently. One such variable that is well established at the bulk scale is the material's density and effective atomic number, which is known to improve the attenuation of X-rays when increased. To investigate if this is consistent at the nanoscale, $LiREF_4$ nanoparticles were synthesized with Y^{3+} and Lu^{3+} acting as the rare-earth (RE) ion in the ternary structure, which allows for variation in the material density and effective atomic number without changing the RE site symmetry, coordination number, or nanoparticle morphology. By incorporating Eu^{3+} as an activator ion, the change in radioluminescence efficiency can be observed through the change in emission intensity from Eu^{3+}. By gaining insight into how the choice of host material impacts the efficiency of radioluminescent nanoparticles, more promising results can be achieved when exploring their potential applications in the future.

One-pot Synthesis and Characterization of Chiral Carbon Dots using Response Surface Methodology and Their Anti-bacterial Properties

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The ongoing social and ecological changes in the past few centuries have negatively affected the lives of all human beings by causing infectious diseases to be one of the leading causes of death. With limited innovations in antimicrobial tools, scientists have turned their attention to nanomaterials that can mimic bacterial-like architectures. Carbon dots (CDots) have garnered significant attention owing to their extremely small sizes (<20nm), ease of fabrication, low cost of production, and unique optical properties. They can be prepared via bottom-up strategies using molecular precursors such as citric acid with the aid of passivating compounds to dope the structure with heteroatoms. One such class of passivating agents is amino acids, which play major roles for microorganisms based on their stereochemistry. While some limited works have demonstrated the antibacterial properties of chiral CDots against different classes of bacteria, CDots from chiral amino acids remain largely unstudied and their mechanism of action is mainly unknown. We report the successful synthesis and characterization of amino acid-derived CDots using microwave synthesis and optimization of the reaction conditions using Response Surface Methodology. Our findings could potentially pave the way for developing novel antimicrobial agents in different applications.

Binary Metal Chalcogenide Templates Direct the Formation of Lead-Free Quaternary Nanocrystals

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Pirquitasite Ag_2ZnSnS_4 (AZTS) nanocrystals (NCs), have emerged as useful materials for photovoltaics due to their tunable optoelectronic properties, as well as the earth-abundance of their constituent atoms. However, the synthesis of quaternary nanocrystals is complicated due to the emergence of undesired unary, binary, and ternary phases, as well as the polymorphic nature of quaternary products. To tackle this complexity, routes involving intermediate binary templates (*e.g.* Ag_2S) and subsequent cation exchange can give access to quaternary phases that are otherwise thermodynamically disfavoured or synthetically challenging. The controlled formation binary templates can be leveraged to attain NCs with improved size dispersity, achieving quantum-confined AZTS emission in the red (λ<750nm) region of the visible spectrum for the first time. We have identified two unreported intermediates in the formation pathway of AZTS nanocrystals, acanthite α-Ag_2S and canfieldite Ag_8SnS_6, which we can manipulate to synthesize ultra-small AZTS particles (d~2nm) with emission wavelengths as short as λ~650 nm.

Covalent IR820-COOH embedded in dense silica shell around LnUCNPs for NIR dye sensitized based Photocatalysis

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NIR Dye sensitization is one of the most effective methods for luminescence enhancement of lanthanide upconverting nanoparticles (LnUCNPs). However, the field remains stagnant due to poor photostability of NIR dyes. With our previous work we modified IR820 with para- substituted different electron withdrawing thiophenol group, to improve its photostability. But even with the modified IR820 dye sensitized LnUCNPs, the luminescence enhancement lasts for limited duration. With this work, we resolve the problem of photo degradation of the NIR dye, by covalently embedding it in the dense silica shell around the nanoparticle. In this work, we optimized the IR820-COOH dye amount for maximum luminescence enhancement. Moreover, on spectroscopically comparing the dye embedded system with electrostatic system, no change in emission of the nanoparticles was observed, owing to protection of the dye from photo degradation. This opens the way to a new field, where covalent dye embedded system can be used for NIR based dye sensitized photocatalysis. This is the first study, where we inserted 15 nm hematite nanoparticles in the wide pore silica shell around the dye embedded covalent system and carried out Fenton type photocatalytic rhodamine B degradation at 800 nm excitation.

POLYMER SCIENCE

Additive Manufacturing of Photoactive Materials

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Polymer processing displays at its core structure-processing-property relationships which is key for understanding the materials' behavior and thus for developing new and more efficient devices. Additionally, additive manufacturing is a new and emerging processing technique that precisely builds objects with an additional dimension via robotic deposition of the material. Although, as useful and promising additive manufacturing is shown to be, there is a lack of understanding of how the process will impact the printed material at the molecular level. Herein we utilize extrusion-based additive manufacturing with the means of developing photoconductive devices. A photoconductive device is one that upon exposure to electromagnetic radiation will change its resistance and can be used in various modern electronic devices. The processing of photoconductive materials has shown to prove that there is molecular change when shear forces are applied to a material during the extrusion process. Systems of polystyrene, polypropylene carbonate and poly(methyl methacrylate) all combined with poly(3-hexylthiophene-2, 5diyl) are evaluated for their printing capabilities in regards to the design of photoactive devices. A system of polyethylene oxide and P3HT is also analyzed via UV-vis spectroscopy to evaluate the impact of the shear forces on the molecular assembly during the extrusion process.

Abstracts – Poster Presentations

ANALYTICAL CHEMISTRY

CE to the ReSQ! Automated label-free capillary electrophoresis (CE) analysis of Asparaginase activity using the “Inject-Mix-React-Separate-and-Quantitate” (IMReSQ) Method

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Asparaginases catalyze the conversion of asparagine to aspartic acid and ammonia and are a common therapeutic enzyme. Current methods for monitoring asparaginase activity include mass spectrometric, chromatographic, and colorimetric techniques. These methods are time consuming, laborious, require µL- mL of sample, require labelling, or have insufficient sensitivity. The established Inject-Mix-React-Separate-and-Quantitate” (IMReSQ) method is an attractive alternative to the methods described above. IMReSQ is a capillary electrophoresis (CE) method that first injects nanolitres of enzyme and substrate, then allows the reagents to mix by transverse diffusion, followed by on-capillary catalysis. The reaction is stopped by applying voltage and separating the substrate, product, and enzyme based on electrophoretic mobility, followed by detection and quantitation. IMReSQ is fast, automated, and label-free method that requires only nL of sample and is compatible with a variety of enzyme- and CE-friendly buffer combinations. Here, we use IMReSQ to monitor the depletion of the substrate, asparagine. By implementing lysine and glycine as internal standards, we can correct for variability in injection and quantitate the analyte. We demonstrate that this method is sufficiently sensitive and accurate for monitoring changes in asparagine concentration. This work lays the foundation for future highly sensitive IMReSQ CE- mass spectrometry experiments.

In vitro metabolism of BPA analogs by LC-HRMS/MS

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Bisphenol A (BPA) is a synthetic compound commonly used in the production of plastics. It was banned in Canada in 2008 due to its adverse health effects. However, the BPA regulation to date does not address its analogs which can be preferred alternatives in the plastics industry. BPA analogs such as bisphenol B (BPB), bisphenol AP (BPAP) and tetrabromobisphenol A (TBBPA) have started to replace BPA in several applications. This study is focused on investigating the potential stable and reactive metabolites generated *in vitro* from these compounds. BPA analogs were incubated with hepatic fractions with different co-factors to study their stable and reactive oxidative metabolites, as well as glucuronide and sulfated conjugates. Samples were analyzed by LC-HRMS/MS on a biphenyl column, with two sets of mobile phases showing very different sensitivities for parent compounds and metabolites. High-resolution MS/MS was used for the investigation of fragmentation pathways of bisphenols and for the structure elucidation metabolites.

INORGANIC CHEMISTRY

Evaluation of hetero-bislanthanides complexes for MRI and optical imaging

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University of Ottawa

Lanthanides are known to have both magnetic resonance imaging (MRI) and optical properties, which make them interesting to explore as multimodal contrast agent. Lanthanides, from europium to lutetium, were used to create hetero-bislanthanide complexes in a controlled 1:1 ratio in order to begin to explore their properties towards their use in application as contrast agents to enzymatic activities or for cell labelling. Both longitudinal and transverse water proton relaxivities were calculated for each bis-lanthanides compound to identify any intresting properties as MRI contrast agents. Optical properties of a combination of some of these lanthanides were also evaluated, with strong fluorescence enabled by the energy transfer of the ligand to the lanthanide ions. The synthesis of the bis-lanthanide molecule is realized first by preparing the 2 individual components followed by an uncatalyzed "click" reaction to produce the desired bislanthanide complex with precise control to yield a 1:1 lanthanides ratio. Absorbance, excitation and emission spectra were acquired on EuGd, EuYb, EuEu and LuLu complexes, where Eu(III) is on the DOTA quinoline moiety. Unexpectedly, the hetero-bislanthanide complexe GdTm showed higher relaxivities even higher than GdGd. With the optical analysis, europium showed a luminescence where its emission is highly dependent of the chemical environment.

Synthesis of Tb(III)-UiO-66 Analogues with Enhanced Photoluminescence

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Over the past few decades, metal–organic frameworks (MOFs) have gathered considerable attention due to their high surface areas, crystalline structures, their chemical compositions as well as the shape and size of their pores. These porous materials are made of metal nodes bridged by organic linkers. Due to the versatility of MOFs, they can be used for different types of

applications ranging from wastewater remediation to biomedical imaging, amongst others. Rare-earth (RE) elements have unique luminescent properties, including narrow emission peaks, large Stokes' shift and long luminescent lifetimes which makes them an interesting choice for incorporation in materials for optical imaging (OI). Using RE elements as metal nodes in MOFs allow for the formation of RE-MOFs that could be utilized for bioimaging. A new series of terbium-based MOFs, based on Tb-UiO-66 are synthesised to study the effect of different linkers on the quantum yield of Tb(III) emission from the MOF. The synthesis, characterization, and photoluminescent properties of each derivate will be presented. The structure and properties of the materials presented are studied using single-crystal X-ray diffraction, powder X-ray diffraction, and photoluminescence measurements including quantum yield. These characterization techniques allow for a better understanding of the structures of each MOF analogue.

Adsorptive Removal of Oxyanions from Water using a Zr-based Metal–Organic Framework

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Concordia University

Oxyanions of various elements are common contaminants in wastewater resulting from industrial processes, mining, and power generation. Zirconium-based metal–organic frameworks (MOFs) have been previously shown in the literature to capture a variety of oxyanions by adsorption on nodal open metal sites, typically binding in an η2μ2 fashion. Herein, the adsorption of a new class of oxyanions on Zr6-based MOFs will be discussed, including the kinetics of adsorption, maximum uptake capacity, and characterization of the adsorption mechanism. The method of nodal binding is investigated by differential pair distribution function analysis (dPDF) and diffuse reflectance Fourier transform infrared spectroscopy (DRIFTS). Additionally, the MOF is tested for its ability for regeneration and potential for multi-cycle reuse, as well as post-adsorption characterization to ensure its stability and suitability for wastewater remediation applications.

Solvent-Free Aerobic Oxidations of Phenols by Copper-Based Catalysis

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Mechanochemical reactions, particularly those involving ball milling, are increasingly being investigated as a means of achieving greener, more efficient, as well as novel reactivity in the absence of bulk solvents. In that context, catalysis under mechanochemical conditions is of particular interest. This presentation outlines our recent work on the development of catalytic mechanochemical aerobic oxidations on phenols, including the synthesis of 1,1'-bis-(2-naphthol) (BINOL) and its derivatives. Specifically, we outline a mechanistic and reaction scope study of a mechanochemical approach for phenol couplings through copper-catalyzed C-H activation. The results reveal that mechanosynthesis of BINOLs and other biphenols can proceed faster and at lower temperatures than in solution. The ability to control the reactivity of such substrates with solid-state catalysis illustrates the significant impact of mechanochemistry in natural product synthesis.

Recycling and Reuse of Solvents for the Synthesis and Purification of Metal–Organic Frameworks

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Concordia University

Metal–organic frameworks (MOFs) are a class of porous materials comprised of organic ligands and inorganic metal nodes, with porosity unlocking their potential for several different applications, from catalysis to drug delivery amongst others. The most common method for synthesizing MOFs includes solvothermal synthesis using the high boiling point solvent N,N-dimethylformamide (DMF). The synthesis is followed by solvent exchange with lower boiling point solvents, such as acetone, to remove impurities from pores and to facilitate the activation process, where the MOFs pores are cleared of solvent molecules. The process of synthesizing and purifying MOFs often results in the use of copious amounts of these solvents for single use, which can be quite wasteful and harmful to the environment. This project explores the effectiveness of using rotary evaporation to distill and recycle DMF and acetone, a procedure that can be easily adopted in most labs. The recycled solvents are then used to successfully synthesize and purify four widely studied d-block metal MOFs, Zr-MOF-808, Zr-UiO-66, HKUST-1 (Cu) and ZIF-8 (Zn). These MOFs are characterized using a variety of techniques, including powder X-ray diffraction, scanning electron microscopy, and nitrogen gas adsorption amongst others.

Electrochemical deposition and conversion of aragonite microstructures into shape-preserving photocatalytic perovskites

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Metal halide perovskites are an emerging class of potentially photocatalytic semiconductors with relatively narrow, tunable bandgaps in the range of many desirable redox half-reactions. Directly synthesized perovskites form orthorhombic lattices that grow into cubic crystals with little freedom to take on other morphologies. Herein, the indirect synthesis of $CsPbBr_3$ using a previously reported metal carbonate cation exchange process allows for the creation of shape-preserving perovskite microstructures. First, the electrodeposition of calcium carbonate microstructures was explored by varying the time of the reaction. The stepwise formation of aragonite crystals allows for a great variety of sizes and shapes used to elucidate the physical changes occurring during the conversion process. When the microstructures are exposed to concentrated Pb^{2+} and CsBr, the outer surface is converted while the core of the crystal remains unchanged. Large crystals do not show changes in elemental or structural analysis post-synthesis because of the thin layer of perovskite on the surface. Shorter deposition times produce

smaller microstructures allowing for a higher ratio of $CsPbBr_3$ compared to the other carbonate phases. A better understanding of the conversion process will allow for the greater development of such photocatalysts in future applications.

Accelerated Development of High Voltage Li-Ion Cathodes

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The need for high energy density Li-ion batteries attracted scientists' attention to high-voltage cathode materials. Among these materials, phosphate polyanion cathode materials ($LiMPO_4$), with ordered olivine structure, are most intensively investigated. However, candidates such as $LiCoPO_4$ have shown numerous challenges generating from poor electronic/ionic conductivities, which cannot be address simply by employing typical solutions such as nanosizing, because it would result in extremely poor cycling performance. Here, high-throughput methods have been applied to develop near-micron sized carbon-coated $LiCoPO_4$ with improved energy density and capacity retention. In total, 1300 materials with 46 different substituents have been synthesized and characterized. A number of substituents show greatly improved capacity (e.g., 160 mAh g^{-1} for 1% In substitution vs 95 mAh g^{-1} for the pristine). However, co-doping is required to improve extended cycling. $Li_{1-3x}Co_{1-2x}In_xMo_xPO_4$ is found to be particularly effective with dramatically improved cycling (as high as 100% after 10 cycles, vs ≈50% in unsubstituted). While In improves the electronic conductivity of the carbon-coated materials, Mo co-doping gives larger particles and DFT calculations show that Mo impedes the formation of Li/Co antisite defects.

PHYSICAL CHEMISTRY

Chirality Induced Spin Selectivity in Contact Electrification

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In electronics, information is typically stored, processed, and communicated using an electron's charge. This model has become increasingly energy-inefficient because movement of charge within an information processing device invariably causes current flow and an associated dissipation. One way to circumvent this issue would be to replace the 'charge' of an electron with its 'spin' to encode information leading to more energy-efficient green electronics. A recent method to create spin filter interfaces relies on the use of chiral molecules through the chirality induced spin selectivity (CISS) effect. CISS surfaces were utilized to exchange charges through contact electrification in triboelectric nanogenerators (TENGs). Contact electrification, also known as triboelectrification, is a phenomenon by which electric charges move between dissimilar materials upon contact. To this end, we demonstrate a TENG device that generates a stable electrical output, where we have monitored the voltage and current under various spin filter conditions. One avenue we have explored for our chiral films is the use of hybrid organic–inorganic perovskites (HOIPs), such as (R-MBA)2CuCl4 and (S-MBA)2CuCl4. Given their high spin polarization, facile synthesis, and thin film preparation by spin coating, we present their use in a TENG to study the CISS effect.

The formation of protein fibers from Tobacco Mosaic Virus (TMV) self-assembling capsids.

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Viruses have become a source of inspiration for the development of hierarchically-structured and responsive materials. Their protein sub-units self-assemble to form intricate capsids, which can be integrated into polymeric materials to produce devices for sensing, nanomedicine, energy, and nanoparticle synthesis applications. The Tobacco Mosaic Virus (TMV) is of particular interest for the development of novel protein-based materials due to the well-characterized self-assembly of its capsid coat protein into disks and rods. The focus of this poster is on our progress towards exploiting this self-assembly to obtain hierarchically-ordered protein fibers. Drying droplet experiments were conducted which showed the formation of free-standing solid fibers. Characterization with small angle x-ray diffraction (SAXS), confocal Raman spectroscopy, and polarized light microscopy (PLM) indicates that the produced fiber has an underlying hierarchical- structure. While further work is ongoing, qualitative observations of its mechanical properties point towards the formation of a novel proteinaceous fiber that is quite different from previous examples of such fibers.

A Comparison of the Physicochemical Impacts of E-Cigarette Additives α-Tocopherol and α-Tocopherol Acetate on Pulmonary Lung Surfactants

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In late 2019, the Centers for Disease Control and Prevention (CDC) started looking into a sharp increase in hospitalizations due to lung injuries associated with vaping. The rise in lung injuries called into doubt the idea that vaping is a better alternative to smoking and piqued the focus of many researchers. The Food and Drugs Act (FDA) has classified many of the vaping components as safe for use, yet the classification has been given for ingestion and not inhalations. Vitamin E acetate from the FDA illicit products, which is used as a thinning agent for vaping solutions, was identified as a potential causative agent of e-cigarette or vaping use-associated lung injury (EVALI), yet the molecular mechanism behind this lung function impairment remains unknown. This work was designed to identify the physicochemical impacts of additives (vitamin E and vitamin E acetate) on the functional properties of model lung surfactant films. The film stability of single additive systems (additive:surfactant) is evaluated using surface pressure-area isotherms and compression-expansion cycles to simulate the breathing cycle. The

film's structural changes are studied using Brewster-angle microscopy (BAM) and grazing incidence X-ray diffraction (GIXD). We also visualized the film morphology of films using atomic force microscopy (AFM).

ORGANIC CHEMISTRY

Mechanistic insight into formal [4+2] cycloadditions of maleimides on duplex DNA.

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The labeling of nucleic acids is crucial for understanding cellular functions and regulations. Copper-free “click” chemistry has emerged as one of the most important strategies for post-synthetic labeling of cellular nucleic acids in vitro and in vivo. Terminal alkenes have recently emerged as minimalistic modifications that can serve as reactive groups in catalyst-free bioconjugation reactions. Herein, we aim to compare the dual-reactivity of 5- vinyl-2'-deoxyuridine (VdU) and 5-(1,3-butadienyl)-2'-deoxyuridine (BDdU) in both inverse- (invDA) and normal-electron-demand Diels-Alder (DA). VdU reacted faster with maleimides (DA) than BDdU, whereas the opposite trend was observed for their reactions with tetrazines (invDA). VdU-maleimide reactions furnished high yielding bioconjugation reactions on duplex DNA in vitro (>90%) and can be applied to fixed-cell labeling. We postulated that the enhanced reactivity stemmed from VdU reacting with maleimides via a formal, stepwise [4+2] cycloaddition whereas BDdU reacted via a concerted [4+2] Diels-Alder cycloaddition. This mechanistic insight has the potential to advance the rational design of future reactive labels for successful bioorthogonal reactions. This presentation will include stereochemical analyses of the cycloadducts, solvent dependent ^{1}H NMR kinetic experiments, and cellular DNA labeling experiments that confirm a highly desirable asynchronous reactivity of VdU towards various dienophiles.

Synthesis of 1-Methylcyclopropyl Aryl Ethers from Phenols using an Alkenylation-Cyclopropanation Sequence

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The synthesis of 1-methylcyclopropyl aryl ethers represents an unsolved problem in organic chemistry. Access to such compounds could enable studies aimed at elucidating the metabolism of aryl cyclopropyl ethers by CYP450s. In this presentation, we will report our results on the development of a method to prepare methylcyclopropyl aryl ethers via the cyclopropanation of the corresponding methylvinyl aryl ethers, themselves obtained by the vinylation of phenols using potassium vinyltrifluoroborates. Optimization of the vinylation reaction to afford the corresponding vinylether will be presented, followed by the substrate and trifluoroborate scope. Then, development of the cyclopropanation reaction will be shown.

Enantioselective transformations of prochiral α-CF_3 and α-SF_5 ketones

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Numerous CF_3- and SF_5-containing compounds have found applications ranging from insecticides to drug frameworks, and to optoelectronics. As such, the development of synthetic methods towards CF_3- and SF_5-molecules is vital. Our group has previously described a regioselective gold-catalyzed hydration to efficiently obtain α-CF_3 and α-SF_5 ketones from their corresponding alkynes. We seek to “escape from flatland” by developing enantioselective transformations of these prochiral α-CF_3 and α-SF_5 ketones, which is currently an underdeveloped area of research. We initially focused on the reduction to obtain each enantiomer of the β-CF_3 and β-SF_5 alcohols using tailored reaction conditions. We will describe the optimization of the enantioselective reduction of α-CF_3 alkynes using biocatalytic and chemical reduction methods. On the one hand, Baker’s yeast has been employed as a green, inexpensive, and air-stable biocatalyst. On the other hand, the organoborane reagent (+)-DIPCl has been successfully adopted. In both cases, both enantiomers were obtained in high enantioselectivity.

Chiral amplification of the conglomerate crystal with temperature control

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Most chiral biochemical building blocks are homochiral, for example, amino acids, nucleic acids, and sugars, which is clear evidence of mirror symmetry breaking. Conglomerate crystallization of achiral molecules is one of the major directions in studying this phenomenon since, in this case, chirality only exists in the solid state. However, slow conglomerate crystallization originating from an achiral molecule typically results in a racemic mixture of chiral crystals. Scientists reported the mirror symmetry breaking and chiral amplification of racemic sodium chlorate conglomerate crystals under boiling conditions (i.e. temperature gradient). The chiral amplification is believed to be a result of Ostwald ripening coupled with enantiomer-specific oriented attachment. To get a better understanding of the mechanism of chiral amplification through conglomerate crystallization, temperature-controlled crystallization experiments of benzil were carried out using a PCR thermocycler, where the temperature can be regulated quickly and precisely. Like sodium chlorate, achiral benzil crystallizes as a conglomerate to form chiral crystals. Our preliminary results show that mirror symmetry breaking and chiral amplification of benzil from acetone are dependent on temperature control during crystallization.

A Medicinal Chemistry Perspective on Fragment-Based Drug Discovery from Hit to Lead

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Fragment-Based Drug Design (FBDD) has been considered as an effective strategy in drug discovery for several decades now. It is a fast and reliable method which aims to develop drugs from initial low molecular weight fragment hits. These fragments are the starting points for designing more potent compounds and screening them allows medicinal chemists to ascertain and quantify the affinity between the fragments and proteins of interest. After identifying and validating the hits, the challenge lies in making these fragments more drug-like by modifying their molecular structure, which includes different fragment-based optimization strategies like fragment linking, merging and growing. Herein, this poster highlights these different medicinal chemistry strategies by using several examples, emphasizing in the importance of choosing the most suitable approach.

Synthesis of pentafluorosulfanylated organic compounds by Kolbe-type decarboxylative electrochemical cross-coupling

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The pentafluorosulfanyl (SF_5) group, first described in 1950 and known as a "super CF_3", presents "extreme" properties that make it attractive in many fields. Methods to synthesize aliphatic-type compounds containing this group are still very limited. To fill this gap, we decided to explore an electrochemical approach based on a Kolbe-type decarboxylative electrochemical cross-coupling since this reaction allows sp^3-sp^3 asymmetric radical cross-coupling. We chose 2-(pentafluoro-λ^6-sulfanyl)acetic acid (**1**) as the source of the CH_2SF_5group. This presentation will describe the optimization and the scope and limitations of the reaction.

Synthesis of Trioxoazatriangulene-Based Covalent Organic Frameworks

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Covalent Organic Frameworks (COFs) are a novel class of materials with ever-increasing interest from researchers for the inherent crystallinity, porosities, and inexhaustible possibilities to engineer their optical and electronic properties by meticulously designing the building blocks. Despite the extensive research over the years on this topic, it remains challenging to synthesize new symmetrical building blocks with which to form COFs. Consequently, there still exists a limited library of COF precursors. Here, we pursue the synthesis of boroxine and imine-based COFs based on trioxoazatriangulene (TANGO) as a planar and symmetric building block. TANGO derivatives have been previously studied as a highly emissive phosphorescent building block and as precursors of semiconducting monolayer 2D polymers; however, to date, no COFs based on TANGO have been realized. Our proposed COFs will be studied for their optoelectronic properties as light-emitting and semiconducting solids. In addition, the developed methodology to synthesize TBpinTANGO and its subsequent palladium-catalyzed Suzuki-Miyaura reactions open endless possibilities to attach functional groups to the TANGO core for further supramolecular assembly, polymerizations, and COF formations.

Blacklight-mediated chloropentafluorosulfanylation of alkenes and alkynes

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Due to its unique characteristics such as high lipophilicity and high electron withdrawing capacity, the pentafluorosulfanyl (SF_5) compound is of great interest in medicinal and pharmaceutical chemistry. Synthesis of aliphatic or vinylic SF_5 bearing compounds is obtained from the atom-transfer radical addition (ATRA) of SF_5Cl, most often activated with triethylborane and traces of oxygen. To further widen the selection of SF_5 products available, our group is interested in other modes of activation SF_5Cl. Herein, we report a novel blacklight-mediated photoactivation of SF_5Cl.

Arabinonucleic Acids Containing C5-Propynyl Modifications Form Stable Hybrid Duplexes with RNA that are Efficiently Degraded by E. coli RNase H

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The promise of the antisense approach to treat a variety of diseases with oligonucleotides and solutions to challenges that have been encountered in their development is attributable to chemical modification of the nucleic acid scaffold. While these modifications have been proven effective, many alter the underlying structure of the hybrid duplex thus rendering it no longer a substrate for RNase H1. In that regard, we have synthesized a novel C5-propynyl-β-D-arabinouridine (araU^P) phosphoramidite followed by its incorporation into oligonucleotides. Substitution of araU^P in dT_{18} homopolymers results in minor stabilization of duplexes formed with RNA when modifications are placed consecutively, while destabilization is observed for duplexes formed with DNA. Moreover, a uniformly modified araU^P 18-mer oligonucleotide was synthesized which increases duplex stability by 34 °C relative to DNA. The modified oligomer exhibits improved nuclease and serum stability when compared to DNA and duplexes formed between RNA and araU^P oligonucleotides are substrates for *E. coli* RNase H. These preliminary results merit further investigation into C5-propynyl modified arabino nucleic acids for potential therapeutic gene silencing applications.

Synthesis of (2-fluoroallyl)boronates from gem-difluoropropenes

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On the one hand, the defluorinative functionalization of allylic fluorides represents an attractive approach for the preparation of various fluorinated compounds containing a fluoroalkene core. The latter is a useful motif in various fields including pharmaceutical science where it is used as a peptide isostere. On the other hand, organoboron compounds have a rich chemistry allowing their transformation into a wide range of organic compounds. Compounds of the general family of (2-fluoroallyl)boronate combines both features, i.e., a fluoroalkene and a boron substituent. The most convenient method to access them rely on a SN2' nucleophilic substitution reaction of allylic fluorides with a boryl nucleophile using a catalytic amount of a transition metal. As a potential alternative, we are working on developing a transition metal-free strategy. Our approach combines the use of a readily available boron source, bis(pinacolato)diboron, and a Lewis base to provide (2-fluoroallyl)boronates products via a defluoroborylation reaction of gem-difluoropropenes. This presentation will discuss the development of this transformation, the scope of the reaction and some transformations of the products generated.

Aldehydes Deoxofluorination Using XtalFluor®

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The synthesis of organic compounds bearing a difluoromethylene unit (–CF2H) can be achieved quite easily with the deoxofluorination reaction. This reaction allows for the conversion of aldehydes (or ketones) into their corresponding CF2H (or CF2) containing molecules. Since their emergence in the 1970s, the most employed deoxoflurorination reagents remain aminofluorosulfurane derivatives, such as DAST and Deoxo-Fluor®. Recently, OmegaChem developed XtalFluor- E®, a novel deoxofluorination reagent exhibiting a crystalline structure. Aside from the high degree of selectivity it offers, this reagent stands out from its predecessors owing to its increased thermal stability and ease of handling, therefore representing a safer alternative to the other, more traditional deoxofluorination agents. Our research group has developed a method for the deoxofluorination of benzaldehyde derivatives, harnessing the potential of XtalFluor-E®. In addition to XtalFluor-E®, an external source of fluoride, Et3N·3HF, is needed for the reaction to proceed. The optimization of reaction conditions, the scope of the reaction and preliminary results on aliphatic aldehydes will be discussed.

MOLECULAR BIOLOGY

Chemically Modified Antisense Oligonucleotides Targeting the C9orf72 Repeat Expansion Found in Amyotrophic Lateral Sclerosis

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Amyotrophic lateral sclerosis is a neurodegenerative disease caused by repeat expansion within the non-coding region of the C9orf72 gene. Both strands are transcribed into long RNA which aggregate as foci in the cell nuclei and are translated into dipeptide repeat proteins in the cytoplasm. Accumulation of the foci and DPRs is toxic to cells within the CNS and leads to progressive deterioration in the patient's health. Antisense oligonucleotides are an emerging class of therapeutics that can be programmed to hybridize to complementary target RNA and either sterically block translation or recruit RNase H endonucleases. Both mechanisms lead to gene knockdown and can be used to reduce the toxic phenotypic effects of the C9orf72 repeat expansion. In this study, we designed a series of ASOs targeting the G- and C-rich repeats. These ASOs were chemically modified to favor translation blockage or RNase H recruitment, increase cellular uptake and stability, and reduce nuclease degradation. The ability of these ASOs to knockdown foci and DPR expression were analyzed by fluorescence in situ hybridization, flow cytometry-based reporter assays, and atomic force microscopy. Overall, these studies provide insight into the genetic cause of ALS and the successful design of therapeutic oligonucleotides to treat this disease.

Effects of lanthanide-doped upconverting nanoparticles on nuclear homeostasis

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Upconverting nanoparticles (UCNPs) can generate high energy photons through the absorption of multiple photons of lower energy through a process known as photon upconversion. Lanthanide-doped UCNPs (Ln-UCNPs) are a class of nanoparticles that have unique physio-chemical properties. These features are ideal for biological and medical applications. Accordingly, Ln-UCNPs have emerged as promising tools for theranostics. However, the bio-nano interactions of Ln-UCNPs are poorly understood. This knowledge gap has limited the use of Ln-UCNPs in living cells. Nuclear homeostasis is essential to cope with stress, such as the exposure to nanomaterials. Our research defines the impact of Ln-UCNPs on cell physiology, as it relates to nuclear biology and stress responses. To this end, we are assessing the effects of Ln-UCNPs on cell viability, the localization and abundance of key components of the nucleus, and the damage to this organelle. Our work provides a quantitative readout for stress responses, proteostasis, and cell organization in Ln-UCNP treated cells. Non-malignant fibroblasts and cancer cells serve as main model systems. Collectively, our experiments determine the biocompatibility and subcellular interactions of Ln-UCNPs. Long-term, this research is expected to generate novel therapeutic and diagnostic tools that can be used for targeted drug delivery and biomedical imaging.

Cellular senescence stabilizes microtubules in intestinal epithelial cells

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Intestinal epithelia are critical to sustain homeostasis in the gastrointestinal tract. Aging promotes intestinal dysfunction through the accumulation of senescent epithelial cells (IECs) in the intestine. To date, the properties of senescent IECs are poorly understood. Here, I developed two model systems to study IEC senescence using two physiologically relevant compounds: butyrate and lopinavir. Butyrate is a short-chain fatty acid that is produced by the gut microbiome. It can also be delivered to the intestine through diet. Lopinavir is an anti-retroviral drug which has been linked to intestinal dysfunction. IECs treated with butyrate or lopinavir developed hallmarks of cellular senescence. Specifically, the treatments reduced cell proliferation, increased lysosomal content, and caused nuclear dystrophy. Using these validated models, I examined microtubule stability by evaluating microtubule disassembly. Results revealed that microtubules become stabilized in senescent IECs. To explore the potential mechanisms, I evaluated the levels of α-tubulin acetylation on lysine-40, histone deacetylase 6, and microtubule-associated proteins. Notably, butyrate and lopinavir employed different mechanisms to stabilize microtubules. In conclusion, my study provides novel knowledge on the physiological changes associated with cellular senescence. I have demonstrated that microtubules are stabilized in senescent cells and that different molecular pathways can promote this stabilization.

A role for the JAK/STAT signaling pathway in mesenchymal stromal/stem cells vasculogenic mimicry.

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Mesenchymal stromal/stem cells (MSC) are believed to be recruited and to adapt within the hypoxic tumor environment of solid tumors, and contribute to the process of vasculogenic mimicry (VM). Without however adopting an angiogenic phenotype, the adaptive molecular mechanisms involved still remain unknown in the formation of these three-dimensional capillary-like structures. Human MSC were cultured in 2D or 3D on a Cultrex matrix mimicking tumor extracellular environment. The formation of 3D structures was digitized, and the images analyzed using Wimasis. Total RNA was isolated to assess gene expression by RT-qPCR. JAK/STAT signaling pathway was assessed using siRNA-mediated gene silencing against STAT3, and pharmacological inhibitors such as AG490, Tofacitinib, and EGCG. Protein lysates were used to assess STAT3 phosphorylation status by immunoblotting. MSC rapidly form capillary-like 3D structures and require the functional JAK/STAT signaling. Snail and Fibronectin, two important components in the process of epithelial-to-mesenchymal transition are induced during VM. Transient gene repression of STAT3 by siRNA also impairs the ability of MSC to form VM. EGCG inhibits STAT3 phosphorylation induced during VM. Pharmacological targeting of the JAK/STAT signaling pathway by EGCG, a polyphenol derived from our diet, may prevent the settling of an alternative process of angiogenesis such as VM.

Yellow is the New Green: Evolution of Old Yellow Enzymes for Sustainable Polymer Production

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Old Yellow Enzymes (OYEs) catalyze the asymmetric hydrogenation of electron-poor carbon double bonds. With a broad substrate range, OYEs are a chief candidate among the need for biocatalysts that can perform asymmetric hydrogenation. This process can create high value chemicals such as biopolymers. Biopolymers are growing in necessity as the world seeks to move away from petrochemical derived plastics and fabrics and toward more sustainably sourced materials. Using a novel, high-throughput assay developed in our lab, we are investigating the activity of a diverse panel of nine OYEs on four polymer precursors to identify candidates for improvement via directed evolution. After purification of the nine candidate OYEs, they will be tested against the four polymer substrates and assessed for activity using our high-throughput assay. Once complete, we select the highest-activity candidate and proceed with directed evolution to further enhance activity and improve stability. Mutant libraries will be generated using structure-guided site-saturation mutagenesis, combinatorial active-site saturation test (CAST) methods, and/or error-prone PCR. Directed evolution will take advantage of known structures where possible. Once mutant libraries are generated, their activity will be assessed, and high-performing mutants will be investigated further. This work will contribute to lessening dependence on fossil fuels.

Investigating the interplay between AMPK and ERK signaling pathways.

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5'-AMP-activated protein kinase (AMPK) is a key player in cellular processes. AMPK controls cell growth, transcription, the response to nutrient limitation or stress, and serves as an energy sensor. At the cellular level, the kinase is activated by the reduction of ATP/AMP ratio. Clinical pharmacological modulators are commonly used to modulate AMPK activity, for example in the context of diabetes or cancer. AMPK communicates with another critical signaling route, the Ras/RAF/MEK/ERK pathway. ERK1/2 (extracellular signal-regulated kinase) are essential kinases that modify a wide variety of protein substrates. Recent work points to a crosstalk between AMPK and ERK1/2 signaling events. The current study investigates the molecular mechanisms that promote this interplay. Specifically, we examine how the pharmacological modulation of AMPK activity affects nuclear homeostasis. Quantitative assays were developed to measure nuclear organization and function. Long-term, this research will provide a better understanding of the network of signaling events that are regulated by the coordination of AMPK and ERK1/2 activities.

Novel fluorogenic DNA intercalators for DNA labeling in living cells

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Bioorthogonal labeling of DNA is a powerful way to learn DNA metabolism in cells and animals, but the click reaction between nucleic acids and reactive tags are sterically hindered by the DNA duplex. Herein, we design a class of novel fluorogenic DNA intercalator. This class of compounds consists of an acridine-orange-like core structure and a tetrazine moiety, which could first intercalate into DNA and perform an inversed electron-demand Diels-Alder (IEDDA) reaction with 5-vinyl-2'-deoxyuridine (VdU) containing DNA in living cells. The close proximity between the vinyl group in DNA and the tetrazine moiety on the probes greatly accelerated the IEDDA reaction in DNA duplex. The loss of the fluorescence quenching tetrazine moiety after the IEDDA reaction also make the reaction highly fluorogenic, which enables imaging of modified DNA even without washing steps. This class of fluorogenic intercalators would enable biorthogonal labeling of DNA in living cells and animals, which would provide insights of DNA metabolism in living cells and animals.

BIOCHEMISTRY

Subcellular localization and membrane topology of AltSLC35A4, a highly conserved alternative protein among vertebrates.

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BACKGROUND: Alternative Open Reading Frames (altORFs) provide a new source of protein diversity in eukaryotes, allowing expression of multiple proteins from a single mature mRNA. The expression of altORFs-encoded proteins (called alternative proteins) has been experimentally validated, and several of them have important biological functions. However, they still largely uncharacterized and have unknown functions. This is the case of the one produced by the double-coding gene SLC35A4, which encodes in its 5'UTR a highly abundant and conserved alternative proteins in vertebrates, AltSLC35A4. OBJECTIVE: To determine the subcellular localization and topology of AltSLC35A4. METHODS & RESULTS: Immunofluorescence revealed that AltSLC35A4 colocalizes with the mitochondrial marker TOMM20 in human cell lines. This result was confirmed biochemically by mitochondria enrichment followed by Western blot. Submitochondrial fractionation using either alkali treatment or selective solubilization of the outer mitochondrial membrane (OMM) with digitonin revealed that AltSLC35A4 is inserted in the OMM. Finally, the topology of AltSLC35A4 was determined using immunofluorescence following differential permeabilization of plasma and mitochondria membranes with digitonin suggesting that the N terminus of AltSLC35A4 is facing the cytosol. CONCLUSIONS: Our study charecterizes molecularly for the first time AltSLC35A4. Future work will focus on the functional interplay between AltSLC35A4/SLC35A4 and eventually other proteins.

Studying TE-mediated macrocyclization control mechanism via saturated mutagenesis of the DEBS-TE.

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Macrocyclic natural products have many useful bioactivities and are thus of interest to the pharmaceutical industry. Such products are difficult synthetic targets due to the challenging nature of macrocyclization, however, nature has found ways to circumvent this. The most common method is through thioesterase (TE) mediated macrocyclization. Despite the fundamental catalytic mechanism being well understood, the control mechanism that dictates macrocyclization over other TE reactivities is poorly understood. Herein, the well-characterized deoxyerythronolide-B (DEBS) TE is studied via saturation mutagenesis of 10 positions to understand this macrocyclization control mechanism further. A total library of 1470 mutants was created to ensure >99% coverage and screened via LCMS, where 10% of the true mutant library is biochemically characterized. Mutations at these 10 positions show a general loss in macrocyclic yields, with L35 and A77 being the least tolerable positions. Product distribution analysis of mutants shows Q176M having a macrocyclization/hydrolysis ratio 2-fold larger than WT. We postulate the larger hydrophobic side-chain of Met sterically blocks water's access to the acyl-TE intermediate and allows intermediate conformational sampling for macrocyclization. The data shown points towards an induced fit model (IF), where DEBS-TE limits water's access to the acyl-TE intermediate to drive macrocyclization.

LC-MS Analysis of Changes in Cranberry Flavonoids in Crops Grown with Endophytes

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Biological control agents (beneficial microorganisms) have shown success in managing growth and pest control of crops. These beneficial microbes (endophytes) have been shown to exhibit biological control through induction of natural products when incubated with plants. We examine the inoculation of two endophytes, bacterium EB37 (Bacillus Venzelisis) and fungi EC5 (Lachnum sp.) with cranberry crops as a means of biological control. Preliminary field evaluations suggested the endophytic microorganisms enhance the cranberries' growth and provided protection from fungal pathogens. We theorize the endophytes have an impact on the cranberries' natural products, specifically the flavonoid group. In the work herein, we present the development of an LC-MS method to analyze flavonoid standards qualitatively from these cranberry samples using a calibration curve. We use an Agilent 1260 HPLC in tandem with an LTQ Orbitrap to separate and identify these flavonoids and analyze the

data with Xcalibur/Compound Discoverer software. We have identified flavonoids in the cranberry extract and will measure their peak areas to examine any changes in flavonoid amounts in the inoculated cranberries.

Assessing target engagement of newly discovered protein RAS binding compounds using cellular thermal shift assays (CETSA).

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The proteins of the RAS family are often mutated in a wide array of different cancer types including bladder cancer. Therefore, they make attractive drug targets due to their implication in tumor formation. Using the fragment based drug discovery strategy (FBDD), our team, in collaboration with NMX Research Solutions Inc., has found new compounds capable of interacting with RAS proteins in vitro. Our next goal is to evaluate the binding potential of these ligands in a cellular context. For this purpose, cellular thermal shift assays (CETSA) will be performed. CETSA involves measuring the thermal stability of target proteins in response to ligand binding in a cellular context. Initial results have been generated in vitro and in the lysate of bacterial cells overexpressing a mutated RAS protein. Lysates from a bladder cancer cell line have also been used for CETSA assays to assess target binding of the new ligands. These results will be useful for evaluating thermal stabilization versus destabilization of the target protein to assess target engagement. Future studies with these ligands might result in the discovery of new therapies with a high degree of selectivity for cancers presenting RAS mutations.

Sumo E3 Ligases identification and characterization through bioinformatics

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SUMOylation is a post-translational modification that allows cells to adapt rapidly to metabolic or environmental changes. This reversible modification on lysines consists of the affixing of a protein called SUMO to a substrate protein via a covalent bond. SUMOylation modifies protein characteristics such as stability and/or inter-protein interactions. SUMOylation is a process that involves the action of three proteins: an E1 to activate SUMO, an E2 to conjugate SUMO and an E3 to direct the E2 enzyme to specific substrates and stimulate catalysis. E3 Ligases are divided into 2 categories: typical ligases containing a RING domain and atypical ligases containing other structural motifs. A protein discovered in 2015, ZNF451, belongs to the latter category. It contains 2 SUMO-interacting motifs that are necessary and sufficient for affixing SUMO to proteins. Our hypothesis is that there are other proteins with E3 Ligase activity through similar motifs. Our approach consists of the bioinformatics identification and characterization of candidate proteins. Our work has already led to the identification of a first candidate, ZNF24. Overall, this study will provide a better understanding of the molecular mechanisms implemented by cells to rapidly regulate many protein properties and could have repercussions in the biomedical and plant biochemistry.

Sequence-Controlled Spherical Nucleic Acids: Gene Silencing, Encapsulation and Cellular Uptake

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Antisense oligonucleotides (ASOs) can predictably affect RNA processing and regulate protein expression; nevertheless, difficulties in delivering these therapies to specific tissues, poor cellular uptake, and endosomal escape have hampered efforts to bring these molecules into clinical use. Spherical nucleic acids (SNAs) form when ASO strands coupled to hydrophobic polymers self-assemble into nanoparticles with a DNA exterior shell and a hydrophobic core. Recently, SNAs have demonstrated outstanding potential as platforms for enhancing the efficiency of ASO cellular uptake and gene silencing. However, no research has yet investigated how the hydrophobic polymer sequence affects the biological characteristics of SNAs. By covalently attaching polymers with linear or branched [dodecanediol phosphate] units and methodically changing the polymer sequence and composition, we were able to construct a library of ASO- conjugates. We demonstrate how these variables significantly impact encapsulation efficiency, gene silencing activity, SNA stability, and cellular uptake, hence proposing optimal polymer structures for gene silencing.

Development of a study strategy of N-glycosylated proteins composing human tears by LC-MS/MS

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Tears are an important component of the eye. Their compositions can reflect the health of this organ, their study is essential. Proteomics having largely contributed to this aspect; few advances have been made in glycoproteomics. The study of glycoproteins can be a challenge, which is why it is important to develop sensitive and robust analysis methods. The aim of this study was to develop an analysis method by LC-MS/MS to study N-glycosylated proteins composing tears. Two glycoprotein enrichment methods were tested, one on hydrazide resin and the other on PBA. Since the study of glycoproteins must also go through a deglycosylation step, two methods were also tested, either by PNGase F or TFMSA. By MS/MS analysis, it was possible to confirm the presence of glycoproteins/glycopeptides. Thus, the methods were evaluated for their ability to identify peptides containing the sequence N-X-S/T and presenting on asparagine's a deamidation (PNGAse F) or a HexNAc (TFMSA). Some of these methods having demonstrated their potentials, these could not only be applied to the study of tears but also for other purposes. Since glycoproteins are known to be good biomarkers, this method could not only be used to study various eye diseases, but also other diseases.

Diversifying chemical modifications on ASOs promoting exon 51 skipping for Duchenne Muscular Dystrophy

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DMD is a fatal neuromuscular disease caused by mutations in the dystrophin gene. The deletion of exons leads to a frameshift in the mRNA and the production of a truncated, non-functional form of the dystrophin protein. Certain exons, 51 and 53, can be additionally skipped and the recovery of a readable frame leads to an internally deleted functional protein. An antisense oligonucleotides (ASO) that base pairs to these exons creates a steric block to the splicing machinery, thereby disrupting splicing and resulting in exon skipping. The design of novel modification patterns containing 2'-OMe, LNA and FRNA with a phosphorothioated (PS) backbone have shown unprecedented skipping levels for exon 53 in human myoblast cells, leading them to be tested *in vivo*, with optimistic results. For exon 51, an the apparition of cryptic splicing products, as well as weak exon-skipping caused more porblems. As an effort to recover the correct splicing product we are pursuing ASOs containing new patterns and combinations of 2'-modified nucleotides. We present data on their binding affinity through T_m experiments, and their activity when administered to immortalized KM155 and in mice. We also describe the synthesis of conjugates in an attempt to enhance their delivery in muscle tissues.

Elucidating the structural dynamics and modification mechanism of Haloduracinβ using Nuclear Magnetic Resonance Spectroscopy

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Lanthipeptides are a class of thioether linkage-containing RiPPs with antibiotic functions. Class II lanthipeptide synthetase HalM2 catalyzes a total of seven dehydrations and installs four thioether rings into its HalA2 precursor peptide substrate. This highly dynamic enzyme has piqued our interest because, while it must possess relaxed substrate specificity to iteratively modify HalA2, the enzyme nevertheless maintains strict biosynthetic fidelity and only installs a single set of thioether rings. It has been hypothesized that a conformational sampling of the enzyme-peptide complex makes important contributions to these properties. We are interested in understanding the biophysical processes guiding the interesting functional properties of HalM2 at atomic resolution using Nuclear Magnetic Resonance Spectroscopy. Accordingly, we have performed a combination of 2D and 3D NMR experiments on isotopically labelled peptide (^{15}N, ^{13}C, ^{1}H) to fully assign the peptide. We observe significant changes in chemical shifts as the peptide is modified by the enzyme. We also performed T1-T2-NOE experiments to study the structural dynamics of the peptide in its unmodified and modified forms. NOE experiments suggest that the leader peptide, which is highly conserved throughout lanthipeptides, has considerable local structure which may help the enzyme to recognize, bind and therefore modify the peptide.

Effects of SUMOylation on protein-protein interactions: development and application in Rett syndrome

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Post-translational modifications can alter a variety of protein-protein interactions in a fast and reversible way. Specifically, SUMOylation can reinforce interactions involved in biological processes ranging from transcription regulation to DNA repair. A growing number of evidence indicates that SUMOylation is crucial to the activity of *Methyl CpG Binding Protein 2* (MeCP2), a transcriptional regulator associated with gene transcription regulation. Various mutations of MeCP2 are known to cause Rett Syndrome (RTT), a neurological disorder occurring in 1/10000 women and leading to severe cognitive and motor impairments. These mutants all share a decrease in SUMOylation caused by a loss of affinity between MeCP2 and a SUMO E3 ligase. In turn, this contributes to a loss of MeCP2's activity and to the severity of Rett Syndrome. Our hypothesis is that we could alleviate some of RTT's symptoms by re-establishing MeCP2's protein-protein interactions through enhancing its SUMOylation. Unfortunately, the impact of SUMOylation enhancements is not well known. This project thus aims to study and characterize the effects of SUMOylation enhancement on MeCP2's protein-protein interactions. The attained results will be able to provide better understanding of the importance of SUMOylation on protein-protein interactions and provide new therapeutical strategies for diseases such as RTT.

Gelsolin aggregation and inhibition: Biophysical characterization

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Gelsolin is an actin-binding protein responsible for the remodelling of the actin cytoskeleton. Under pathological conditions, Gelosolin is susceptible to aberrant proteolytic cleavage. The D187N and D187Y point mutations have been associated with fragmentation, causing the formation of amyloidogenic 8kDa (173–242) and 5 kDa (173–225) fragments. The fragments systematically deposit within the organs to promote cell death. Wildtype peptides within the same sequence do not demonstrate similar aggregation propensity or amyloid formation. Gelsolin protein is also capable of propagating a diseased state across cells through the process of seeding. Despite the detrimental effects of Gelsolin mutation, the mechanism of amyloid formation is understudied. Herein, we investigated the aggregation propensities, inhibition, and morphology of wild-type Gelsolin peptides (187-193) and their associated mutants under physiological conditions. We also explored the seeding reaction of Gelsolin with high-concentration mutant peptides to monitor the propagation of the diseased state. Spectroscopic and microscopic methods allowed for the identification and visualization of aggregates and amyloids. We reported that CFILDL-containing peptides were prone to aggregation, which may be inhibited and reversed with small molecules. The seeding of Gelsolin peptides promoted aggregation and fibril formation. Of note is the unique behaviour of peptide mutants with respect to their aggregation.

La SUMOylation des facteurs du chocs thermiques (Hsfs) chez Arabidopsis thaliana

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La SUMOylation est une modification post-traductionnelle des protéines qui permet aux plantes de répondre de rapidement à des stress abiotiques comme la déshydratation ou l'exposition à des température extrêmes. La SUMOylation des protéines est typiquement dépendante de la présence de sites de SUMOylation (motif YKxE où Y est un résidu hydrophobe, K la lysine ciblée par la SUMOylation, x un résidu quelconque et E un glutamate) sur ces protéines. Du fait de leur très petite taille, les sites de SUMOylation peuvent rapidement apparaître ou disparaître au cours de l'évolution sous l'effet de simples mutations de substitutions. Notre hypothèse est que des changements au niveau de l'abondance et de l'emplacement des sites de SUMOylation, bien qu'ils puissent contribuer à court terme à des instabilités des réseaux protéiques, contribuent à plus long terme à une adaptation rapide des plantes à de nouveaux environnements. Notre objectif est ainsi de fournir une perspective évolutive quant aux rôles de ces mutations. Plus précisément, nous déterminerons les conséquences fonctionnelles d'une augmentation ou d'une diminution du nombre de sites de SUMOylation chez les protéines Hsfs impliquées dans la réponse aux chocs thermiques chez Arabidopsis thaliana, la plante modèle en biologie. Ceci se fera au moyen d'approches bio-informatiques, biochimiques et via la caractérisation de plantes mutantes.

Activity and inhibition of trimethoprim resistant enzymes: insights into evolutionary origin

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Antibiotic resistance is a global threat to public health that has emerged soon after the introduction of antibiotics due to increased evolutionary pressure. One such example is trimethoprim (TMP) resistance conferred by type B dihydrofolate reductases (DfrB, Ki > 1 mM). TMP is a synthetic antibiotic introduced in the 1960s. DfrB show no sequence or structural similarity with bacterial dihydrofolate reductases. DfrB form a unique binding tunnel by homotetramerization of monomers consisting of SH3 domains, which are thermoresistant (activity is restored after heating at 95°C). Inhibitors that selectively target DfrB have been developed. Even though they have suboptimal affinity (Ki ~ 2-20 µM), they can be used to probe the binding mechanism of putative DfrB homologs (DfrBH) identified in metagenomic searches. Those newly identified DfrBH harbor extracatalytic domains of different sizes and were characterized by biophysical methods (termostability assays) and inhibition assays. Results indicate that DfrBH are inhibited by known DfrB inhibitors but their thermostability decreased according to the size of the extracatalytic domain. This is consistent with an evolutionary relationship between DfrB and DfrBH. This increases our understanding of the TMP resistance mediated by DfrB and DfrBH, thus contributing to inhibitor development.

Implementation of the proximity biotinylation approach (BioID) to identify protein complexes associated with RNF13

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Proteins can influence their functions through interactions between them, within signaling systems and pathways. The RING finger domain protein 13 (RNF13) is an E3 ubiquitin ligase, with great implications for learning, memory, and cognitive disorders. However, the majority of his functions remain unknown. This project aims to identify and characterize protein complexes and neuronal signaling pathways associated with RNF13. To identify protein complexes physiologically relevant to RNF13, we used a proximity biotinylation technique using a biotin ligase fused to RNF13. To date, the stable expression of the RNF13-UltraID fusion transgene in Neuro2A cell lines (and UltraID control lines) has resulted in different biotinylated-protein profiles for our RNF13-UltraID tool when compared to control conditions. RNF13-UltraID fusion protein (UltraID is a more active and smaller ligase than BioID2) exhibits a higher specific labelling rate in Neuro2A cells compared to results previously obtained with our initially generated tool (RNF13-BioID2). By immunofluorescence, the localization of the RNF13-UltraID fusion protein is identical to wild-type RNF13. The project still requires optimization (labelling time, cell quantities) to obtain quality results and identify protein complexes and neural pathways associated with RNF13.

The role of the SLC35A4 gene in the Integrated Stress Response.

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Introduction: The integrated stress response (ISR) allows cells to adapt to cellular stress such as oxidative stress (OS). The ISR causes the general inhibition of mRNA translation. However, the translation of some mRNAs is maintained or increased, to produce proteins essential for the response to OS. The SLC35A4 gene encodes two proteins: SLC35A4, a CDP-ribitol transporter in the Golgi, and AltSLC35A4, a highly conserved alternative-protein of unknown function ubiquitously expressed in mitochondria. Interestingly, previous ribosome profiling studies indicated that in sodium arsenite (OS) induced stress, SLC35A4 mRNA escapes translational inhibition, and the sequence encoding SLC35A4 undergoes the largest increase in translational efficiency out of all cellular mRNAs while AltSLC35A4 translation is maintained/Hypothesis: SLC35A4-encoded proteins play a significant role in the ISR/Objectives and methodology: 1/Validate that the expression of SLC35A4 increases in response to stress, by peptide absolute quantification using mass spectrometry, in sodium arsenite treated 143B cells.2/Test the importance of SLC35A4/AltSLC35A4 in resistance to and/or induction of OS in 143B cells. We used CRISPR/Cas9 to knock-out SLC35A4 and fluorescence microscopy to quantify stress severity/conclusion: This project will determine the role of SLC35A4 in ISR than its relationship with AltSLC35A4, which may have therapeutic potential in various diseases involving the stress.

Metabolic reprogramming reveals a role for the G6PC3 and solute carrier family 37 SLCA2 / SLCA4 components upon the acquisition of a brain cancer stem cell molecular signature

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Background: Glioblastoma multiforme (GBM) is adults' most common malignant brain tumor. GBM cells have an altered glucose metabolism, among which metabolic reprogramming that involves the glucose-6-phosphatase (G6Pase) system has been inferred. Objective: We questioned what roles components of the G6Pase system have upon acquiring a brain cancer stem cells (CSC) chemoresistance phenotype. Methods: Total RNA extracted from four brain cancer cell lines and cDNA arrays were used to assess gene expression by RT-qPCR. Three-dimensional neurosphere cultures were generated to recapitulate the CSC phenotype. In silico analysis of transcript levels in GBM tumors was done by GEPIA. Transient siRNA-mediated gene silencing was used to assess the impact on TNFa-induced inflammation and TGFb-induced epithelial-to-mesenchymal transition (EMT). Results: in-silico analysis of GBM revealed a significantly higher expression in G6PC3, SLC37A2, and SLC37A4. The expression of these genes was further found elevated in U87, U251, U118, and U138 GBM cell models compared to the HepG2 hepatoma cells. G6PC3 and SLC37A4 levels induced in CD133-positive neurospheres. Silencing the genes altered TNFα or TGFβ signaling. Conclusion: Components of the G6Pase system appear to contribute to metabolic reprogramming involved in acquiring a brain CSC phenotype. Such molecular signature may support their role in cell survival and chemoresistance.

Identification of selective glycosyltransferase inhibitor molecules targeting cell-surface fucosylation

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In cancers, increased fucosylation of cell surface glycans is a trademark of malignant cell transformation and contributes to many abnormal cellular events during cancer development. Such increase in the attachment of fucose sugar residues is a result of the abnormal upregulation of specific fucosyltransferase enzymes (FUTs), for example, FUT5 acts to form Sialyl Lewis X, a member of the Lewis antigen family that when overexpressed, is related to advanced tumors, high metastatic potential, and worse prognosis of colorectal cancer. The role that this enzyme plays in the progression of cancers to metastatic stages makes it an attractive target for potential anticancer drugs. In order to quantify activity and inhibition of FUT5, we have developed a high-throughput assay that makes use of a fluorogenically labeled oligosaccharide as a probe of fucosylation. It consists of a 3'sialyl-N-acetyllactosamine-resorufin (3'SLN-Res), which is recognized and hydrolyzed by specific glycoside hydrolase enzymes to release fluorescent resorufin. However, if the probe is fucosylated prior to treatment with glycosidases, they cannot act on the substrate and release of a fluorescent signal does not occur. Using this assay, we aim to test a library of 4,000 small-molecule drug-like compounds in an automated high-throughput screening.

Investigation of the unique structural elements and catalytically important dynamic regions of the Nisin biosynthetic enzyme NisC

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Ribosomally synthesized and post translationally modified peptides (RiPPs) are structurally diverse natural products that often possess potent antimicrobial properties. The widely-used food preservative, Nisin, possesses intramolecular thioether linkages which are critical for its bioactivity. Modification of the precursor peptide NisA to bioactive nisin, is catalyzed by enzymes NisB and NisC. NisB catalyzes dehydration of serine/threonine residues in NisA and NisC catalyzes thioether ring formation, with precisely controlled regio- and stereospecificity. Previous studies have demonstrated how the presence of thio-ether linkages increase the stability and bioactivity of RiPPs. Furthermore, the genetic encodability of RiPPs and the relaxed substrate specificity of the biosynthetic enzymes make them promising candidates for engineering of novel drugs. However, the mechanistic details that regulate the peptide modification remain unclear. In this research, our goal is to better understand the molecular mechanism and the biophysical interactions involved in the cyclization process. Towards this goal, we have developed a mass spectrometry based assay to monitor the NisC activity under *in vitro* conditions. Moreover, hydrogen deuterium exchange mass spectrometry studies of NisC in the presence and absence of NisA revealed a potentially novel leader peptide binding motif and other interesting structural elements which will be further investigated with mutational studies.

COMPUTATIONAL CHEMISTRY

Towards Rapid Computational Screening of Metal-Organic Framework Candidates for Chemical Adsorption of Small Toxic Molecules

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The design of advanced materials for the capture of toxic chemicals is essential due to the tremendous threats the latter may pose to human health and the environment. Metal-organic frameworks (MOFs) have emerged as a promising category of sorbent materials for the capture of such toxic chemicals. However, no clear and comprehensive relationships have been established between the capability of the MOFs to capture toxic chemicals and their structural and chemical characteristics, which limits the rational design of MOFs for that purpose. Accordingly, density-functional theory (DFT) is used to investigate the possible

correlation between the adsorption performance of some MOFs for target molecules and their structural features, such as the nature of the transition metal sites. The magnetic properties of the MOFs are investigated along with their impact on the material bandgap and target molecule adsorption, and an efficient, yet rigorous, DFT strategy is developed, based on primitive unit cell calculations with Hubbard U corrections, to allow for rapid screening of MOFs with different metal sites. The coordinatively unsaturated metals of the MOFs are the most likely sites for chemical adsorption of the target molecules, and the effects of different metals on the adsorption of the target molecules are investigated.

Towards Repurposing of Prescription Drugs as Potential Inhibitors of Botulinum Neurotoxin Metalloprotease

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Botulinum toxins (BoNT) are some of the most lethal, naturally occurring neurotoxins known to humans, causing flaccid paralysis. To reduce respiratory and muscular paralysis, the most potent BoNT serotype A has been the key target of drug design to promote acetylcholine release from the presynaptic membranes. Drug repurposing is a viable strategy to accelerate drug discovery. Hence, the possible inhibitory action of FDA-approved drugs against the BoNT/A metalloprotease is investigated by drug-likeness and Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) properties screening, high throughput virtual screening (HTVS), molecular docking, and molecular dynamics (MD) simulations. The initial drug library contains over 9,000 compounds, and of the 92 drugs identified by HTVS, three are found to have high affinity for the BoNT/A metalloprotease binding pocket, and their interaction with the protein is further investigated by MD simulations. The relative stability of the resulting protein-ligand complexes is confirmed by inspection of structural properties over the 100-ns simulation timescale and rationalized in terms of intermolecular interactions between the drug compound and the metalloprotease binding pocket residues. Our findings suggest FDA-approved hyperlipidemic inhibitors as potential repurposed drug candidates for BoNT/A metalloprotease inhibition and possibly as effective treatments to reduce the effects of BoNT/A intoxication.

NANOCHEMISTRY

From Structure to Function: Bottom-up Fabrication and Individual Characterization of Metamaterials with Resonances in the Visible Regime

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The controlled fabrication and characterization of nanoscale plasmonic structures is a major challenge in the development of next generation metasurfaces and 3D metamaterials. Controlling the geometry of their sub-wavelength components, or meta-atoms, as well as their spatial arrangement can produce materials with highly unusual electric permittivity or magnetic permeability profiles. Using biological scaffolds, such as the tobacco mosaic virus coat protein (TMV), opens up an economical and programmable way to fabricate a broad range of these structures through the tuning of amino acid substitutions, assembly conditions, and the choice of plasmonic components. , We have successfully fabricated and purified individual plasmonic gold nanoparticles (AuNPs) onto TMV in different geometries, including rod-like assemblies, nanotubes, and hexagonally packed and square-packed sheets. The characterization of each individual structure is not trivial, however, due to the heterogeneity in assembly and size of the nanostructures in solution, with each contributing differently to the UV-Vis spectra recorded. By employing dark field scattering microscopy in correlation with transmission electron microscopy, we have been able to isolate different structures' spectral fingerprint to better understand and model each assembly structure's interaction with light.

Design and Characterization of Self Assembled Spherical Nucleic Acids for Gene Silencing

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Nucleic acids therapeutics hold great promise in treatment of classically undruggable diseases, by targeting protein production as opposed to function. However, nucleic acids suffer from hurdles including poor stability, immunogenicity, and poor biodistribution. Spherical nucleic acids (SNAs) have emerged as a class of nanocarriers aiming to improve these shortcomings, and better deliver therapeutic nucleic acids. Self assembled SNAs show promise as delivery vehicles owing to their ease of synthesis, relying on direct conjugation of a series of hydrophobic monomers to a growing nucleic acid strand. This strand can then self assemble into a spherical structure with favourable bio distribution, and the ability to carry small molecule therapeutic cargo. Further iterations on this structure including backbone and base modifications, have shown the ability to use these structures for gene silencing. However, little is known about the stability of self assembled SNAs in response to biological barriers such as changes in pH, salt concentration, and exposure to serum proteins, all obstacles that can impede function and slow transition to the clinic. Herein we demonstrate the stability of phosphorothioated self assembled SNAs to biological barriers, and showcase the need for a stable spherical morphology that can disassemble for gene silencing applications. We also look show unaided uptake into both 2D and 3D tumor spheroid cell models, and probe the mechanism for cellular uptake. SNAs offer a promising platform for delivery of nucleic acid therapeutics due to a combination of enhanced biological stability, simplicity in design and ability to natively enter cells.

Barcoding DNA Nanostructures for High Throughput Cellular Uptake Studies

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Nucleic acid therapeutics (NATs) have shown a new way of treating disease by targeting the gene of interest directly. It is highly specific and presents the possibility to treat any disease with a genetic component. The major roadblocks to the translation of NATs to the clinic are their limited stability and inefficient in vivo delivery. DNA nanostructures are an excellent system to carry and deliver these therapeutics in vivo owing to their biocompatibility, stimuli responsiveness, and the ability to precisely control the physical properties (size, shape, surface ligands, etc.) of these nanoparticles. It has been seen that the physical properties of nanoparticles influence their biological behavior. Therefore, there is a need to systematically study these nanostructures in vivo to obtain precise structure-activity relationships. But, present methods and workflows are tedious and time-consuming as it involves studying each structure one by one. Here, we propose a high throughput method that involves the assembly of our DNA nanostructures with a unique DNA barcode for each structure. This will allow us to screen many nanostructures simultaneously in the same animal. Thus, it will reduce the time needed to study each structure significantly and allow us to extract important design rules for these structures.

DNA-based Strategies for Effective Therapeutic Delivery

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While small molecule drugs are used to target diseases at the level of the protein, nucleic acids, such as anti-sense oligonucleotides (ASOs), are used instead as “up-stream therapeutics” that modify the translation of an mRNA sequence into its protein. When nucleic acids are delivered as therapeutics, they are commonly delivered in association with a therapeutic nanocarriers to shield them from enzymes, known as nucleases, that are responsible for degrading these nucleic acids. But, despite nucleic acids displaying strong therapeutic capabilities, the main obstacles faced with nucleic acid therapeutic delivery is the precarious stability of DNA nanocarriers in-vivo, as well as difficulties in delivering these therapeutics to the appropriate cell environments in the body. To address these drawbacks, I devise a strategy to covalently cross-link the hydrophobic cores of spherical nucleic acids (SNAs), a type of nucleic acid therapeutic nanocarrier. This would aim in improving the stability of our DNA nanocarriers in circulation so that they are not disassembled by various serum proteins. Moreover, I employ the use of hydrophobic dendrimers that selectively bind albumin to modulate the biodistribution of nucleic acid therapeutics. so that they can reach the parts of the body where therapeutic action is needed. Albumin is the most prominent serum protein and is inherently responsible for binding small molecules, hormones, and drugs to circulate them all around the body. Therefore, I seek to improve the biodistribution of my nucleic acid therapeutic constructs by selectively binding them to the albumin in the serum which will subsequently improve the nanocarriers’ circulation, and thus its biodistribution.

Automated Assembly of DNA Wireframe Nanotubes Characterized via Single-Molecule Fluorescence Microscopy

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DNA nanotechnology has revolutionized our ability to position matter at the nanoscale. Despite the widespread use of DNA in materials science, the preparation of custom DNA-based architectures is often time-consuming. A fully automated method to produce sequence and size-defined DNA nanotubes was created. Controlled positioning of non-covalent building elements by programming the sequential addition of desired building blocks yields complex DNA nanostructures where the total number of possible constructs increases as a power function of the number of differing rungs available. Using single-molecule fluorescence imaging and exploiting automation, the kinetics and yield of each synthetic step can be quantitatively determined. This procedure facilitates the iterative improvement of assembly parameters and reveals differences in assembly dynamics with distance to the support surface, as the nanotube is built up from the solid support. In this presentation, I will address the generalizability of the single-molecule-based platform, describe ongoing efforts toward increasing the robustness of our DNA-based nanoassemblies and describe new directions toward assembling architectures for biosensing.

Catalytic Conversion of Polysulfides by Atomic Layer Deposited Titanium Nitride for High-Rate Lithium Sulfur Batteries

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In this research study, a novel catalyst material titanium nitride (TiN) for sulfur cathodes is developed through the use of atomic layer deposition (ALD). The synthesized ALD-TiN catalyst demonstrates controllable ultrafine particle size (< 2 nm) and uniform distribution at nanoscale in the carbon matrix. Combined with electrochemical analysis and multiple post characterization techniques, ALD-TiN demonstrates remarkable catalytic effect to enable the nucleation and deposition of Li2S, which successfully suppresses the dissolution and shuttle of polysulfides. The as-prepared sulfur cathodes with the assistance of TiN catalyst display excellent cycling performance at high rate (4 C) and produce 200% higher discharge capacity than the pristine S-C cathodes.

POLYMER SCIENCE

Apple Pectin based Hydrogel Electrolyte for Energy Storage Applications

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With the increase of portable power sources demand, new technologies, e.g. wearable and flexible electronics, are projected to generate $1.25 billion market by 2022. New storage energy devices are more than ever in demand which requires new specifications: minimizing the environmental impact in the whole battery life cycle, from conception to degradation of the system, and reducing production costs. Polymer hydrogel electrolytes are one of the promising alternatives for processing new flexible batteries. Nevertheless, the original polymers used in these systems don't consider the cost of the environmental impact and safety due to the processing or biodegradability of those hydrogels. In this study, we report a new hydrogel-based electrolyte material made of apple pectin. This presentation will mainly focus on the interactions between pectin functional groups, water, and ions using solid NMR spectroscopy. Thermal properties will be discussed based on thermogravimetric and differential scanning calorimetry analysis. Electrical and electrochemical properties obtained by electrochemical impedance spectroscopy, and galvanostatic cycling, will demonstrate the applicability of such hydrogel electrolytes. This study could promote a great innovation in the energy storage field, by recycling one of apple peel's components (which is the main waste in preserves manufacturing) into a hydrogel electrolyte.

Polymer Matrix Mediated Assembly of P3HT Nanowires

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The properties of a material do not only depend on its intrinsic characteristics but also on its structural organization, which itself is influenced by the way it is processed. In the literature, doped organic semiconductor polymer such as poly(3-hexylthiophene-2,5-diyl) (P3HT), shows a good electrical conductivity in the form of nanowires. However, conventional processing techniques, such as spin-coating, usually leads to low level of nanowires orientation, and thus poor electrical properties for energy efficient applications. By using a non-traditional method, three-dimensional (3D) printing, and more specifically direct-ink writing, we will explore if the alignment of P3HT nanowires can be enhanced via the shear forces experienced during the printing process. To facilitate the processing of the P3HT nanowires, the latter will be blended in a dielectric polymer matrix. We hypothesize that the phase separation between the polymer matrix and the nanowires, combined to the shearing forces experienced upon extrusion, will optimize the alignment of the nanowires, thus leading to enhanced charge transport properties. The properties of the 3D printed materials will be characterized using UV-visible spectroscopy, differential scanning calorimetry and atomic force microscopy. Structure-processing-property relationships will be established to improve our ability to predict and control the 3D printing of pi-conjugated materials.

Understanding solid polymer electrolytes through hot melt extrusion additive manufacturing

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Polymer processing is a mature field of material science which studies the change in properties of materials during and after being processed by a specific method. Yet, there is still a lot to learn in terms of polymer additive manufacturing (AM). The core of the Laventure Lab studies the structure – processing – property relationships to understand the fundamentals of each material used in an AM process. Hereby, we demonstrate how our research is working towards a better understanding of ionic conducting polymers through Hot Melt Extrusion 3D printing. The main advantages of AM as a manufacturing technique can be summarized as rapid prototyping of complex architectures unobtainable with conventional processing techniques. However, to properly understand how the materials behave during extrusion it is primordial to have a proper understanding of the rheological and thermal properties of each material. The liberty of conception and the flexibility of 3D printing allows the design of new architectures and study of physical and chemical properties of the resulting materials. Therefore, an in-depth understanding of the thermal, rheological, and electrochemical properties of polymers used as solid electrolytes will help us lead the way to a more versatile manufacturing path through AM of polymer matrices.

Development and Optimization of Highly Reflective Electrospun Poly(oxymethylene) Nanofibers

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Electrospun nanofibers are unidimensional nanomaterials prepared by applying a high electric field to a polymer solution. These fibers are attracting considerable interest thanks to their ease of processing and their mechanical and optical properties, which are often far superior to those of the corresponding bulk polymers. Using advanced spectroscopic methods, our research group has attributed these improved properties to a very high molecular orientation. Recent works have also shown that a limited number of polymers exhibit, under certain conditions, unusual and particularly intense optical responses caused by quasiparticles called surface polaritons. In this context, we developed, characterized, and optimized highly oriented electrospun nanofibers with a polaritonic response. The fibers were prepared from polyoxymethylene, a robust polymer known for its ability to generate surface polaritons. The fibers' optical response was monitored by polarized specular reflection infrared spectroscopy and optimized through a variety of fiber post-treatments, namely traction, compression, immersion in a refractive index-matching liquid, and drenching in a non-solvent. As a result, their reflectance was improved from around 3% to 60% reproducibly while

exhibiting excellent polarization contrast. This work guides the preparation of polymer materials with unique optical properties and stimulates their application, notably in the field of remote sensing.

Polymer additive manufacturing for antimicrobial materials

R. Zidani*, N. Blanc, M. McGeehan, M. McNeil, A. Laventure
Université de Montréal

Additive manufacturing (AM) has revolutionized the development of functional materials thanks to its ease of use, cost and time efficiencies, reproducibility and tunability. AM is applicable to various materials with the possibility for complex architecture designs. It gives an excellent control on the preparation of functional materials by the robotic nature of the process which makes it more reliable than conventional preparation methods. Application of AM on polymers allow alteration of their properties by additives such as antimicrobial agents. Direct-ink writing (DIW) and digital light processing (DLP) techniques are herein considered for the fabrication of three-dimensional antimicrobial materials. In this work, we present the optimization of the printing process for multiple polymers (thermoplastic, elastomeric and resins matrices), as well as the insertion of photosensitizers as antimicrobial agents. Photochemical analysis performed were also able to inform on the influence of the presence of additives in the material. Pending rheological characterization for printability studies and print fidelity assessment, along with biological assays, these architectures could be very promising options for 3D printed architectures prepared from functional polymers.

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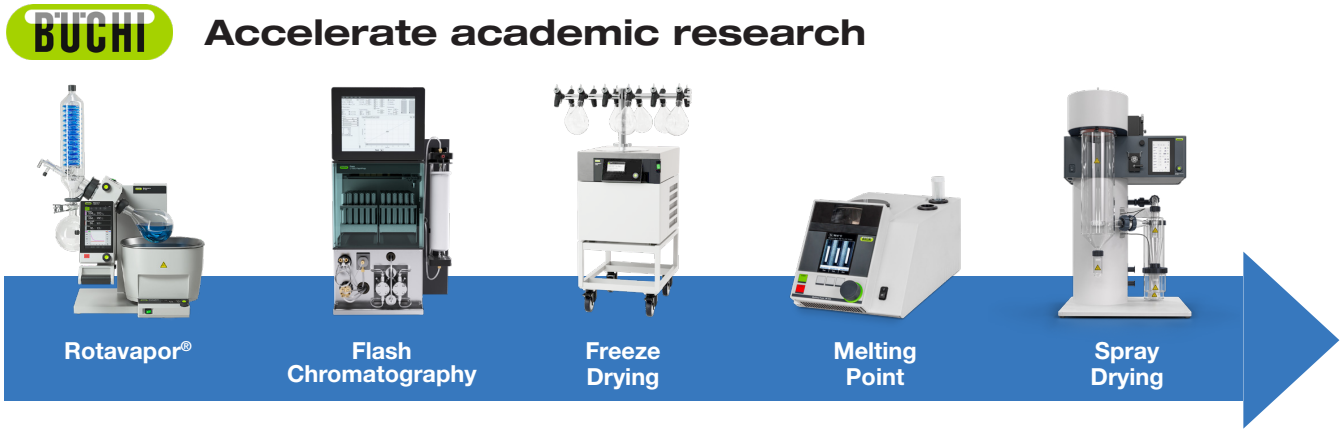
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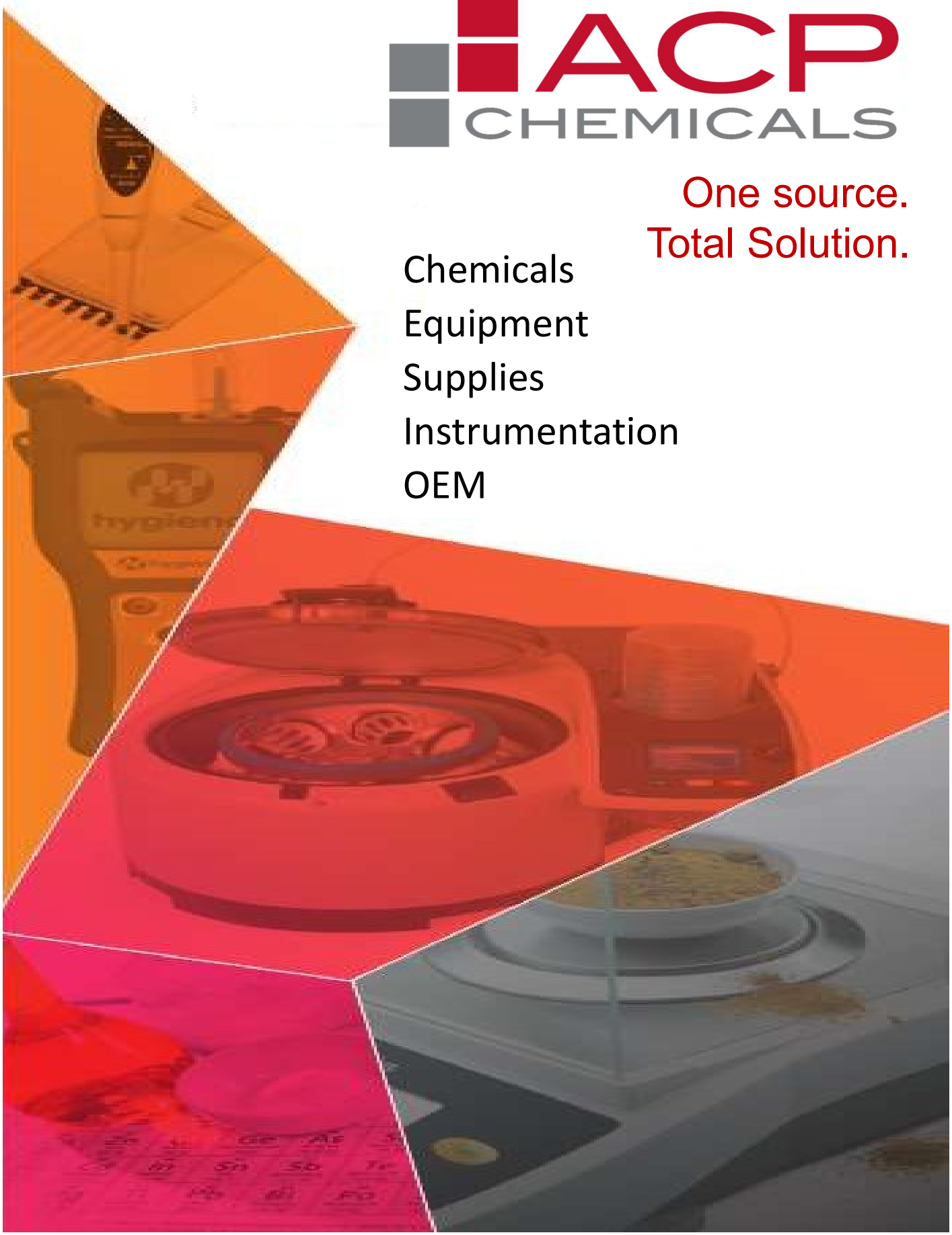
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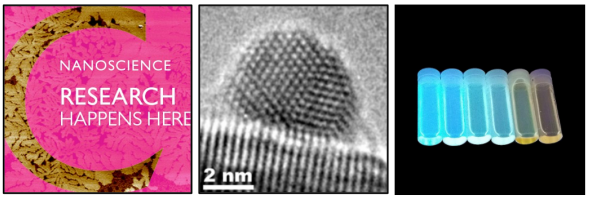

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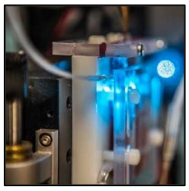
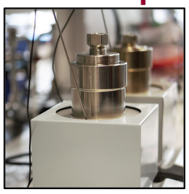
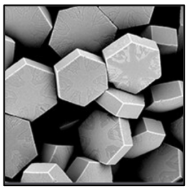

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The CBGRC Organizing Committee

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