UNIVERSITE Concordia UNIVERSITY

26TH ANNUAL CBGRC

Chemistry & Biochemistry Graduate Research Conference

November 29th, 2024

THERAPEUTIC ADVANCEMENTS:

Solutions for global health challenges

Keynote speakers

Dr. Yvan Guindon
Director, Bioorganic Chemistry unit, IRCM

Dr. Karine Auclair
Professor of Chemistry, McGill University

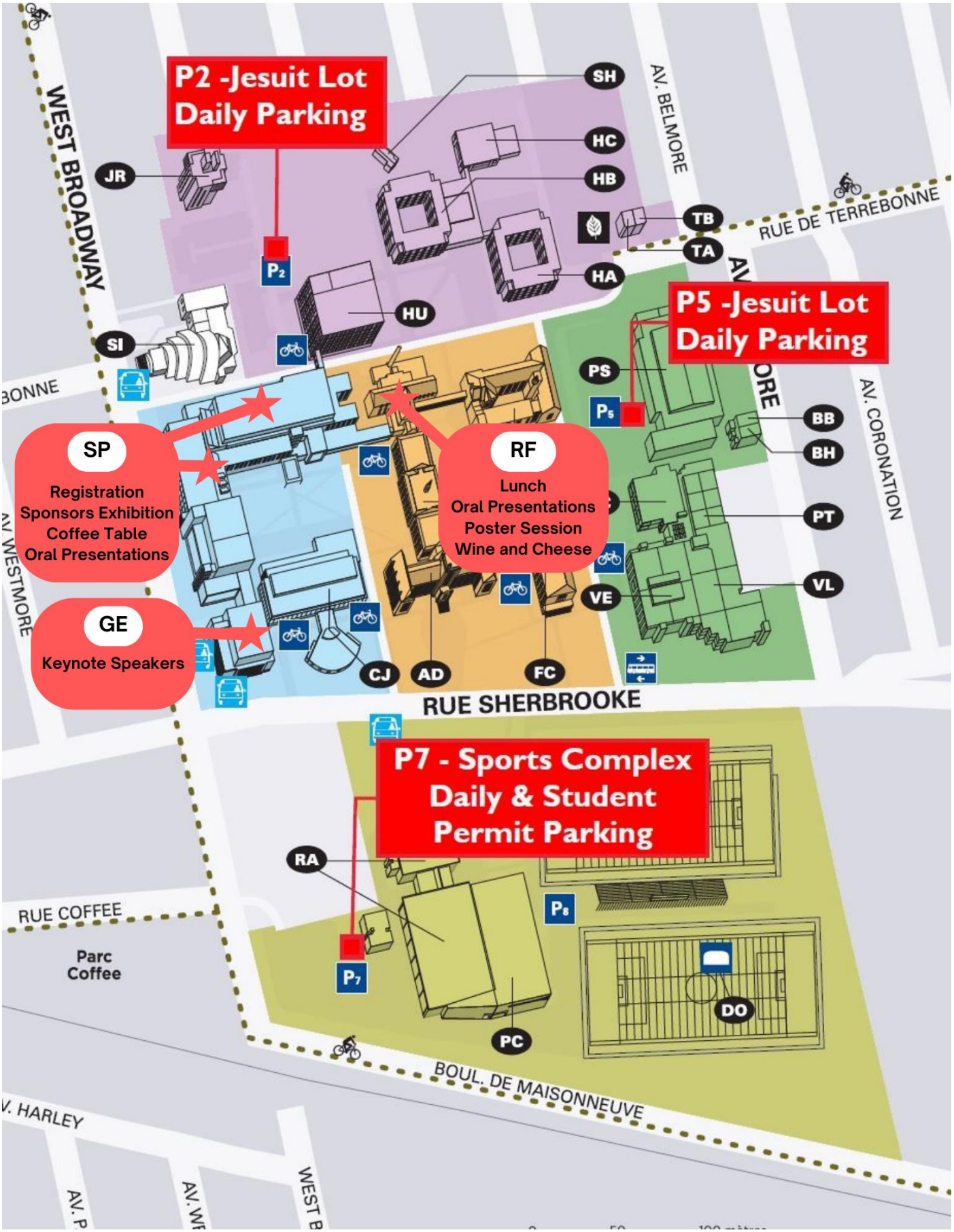
Registration deadline

November 1st 2024

www.concordia.ca/cbgrc CBGRC @cbgrc_annualconference

Table of Contents

Campus Maps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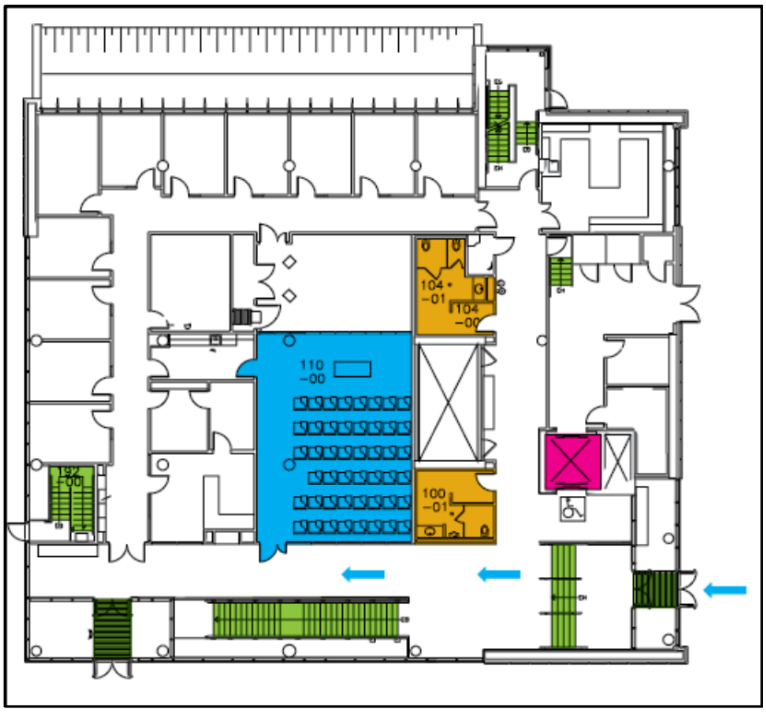
Daily Parking
P5 -Jesuit Lot
Daily Parking
P7 - Sports Complex
Daily & Student
Permit Parking
SP
Registration
Sponsors Exhibition
Coffee Table
Oral Presentations
RF
Lunch
Oral Presentations
Poster Session
Wine and Cheese
GE
Keynote Speakers
WEST BROADWAY
AV. BELMORE
RUE DE TERREBONNE
AV. CORONATION
AV. WESTMORE
RUE SHERBROOKE
RUE COFFEE
Parc
Coffee
BOUL. DE MAISONNEUVE
V. HARLEY
SH
HC
HB
TB
TA
HA
HU
JR
SI
PS
BB
BH
PT
VL
VE
CJ
AD
FC
RA
DO
PC

GE 110



Elevators | Stairs | Washrooms

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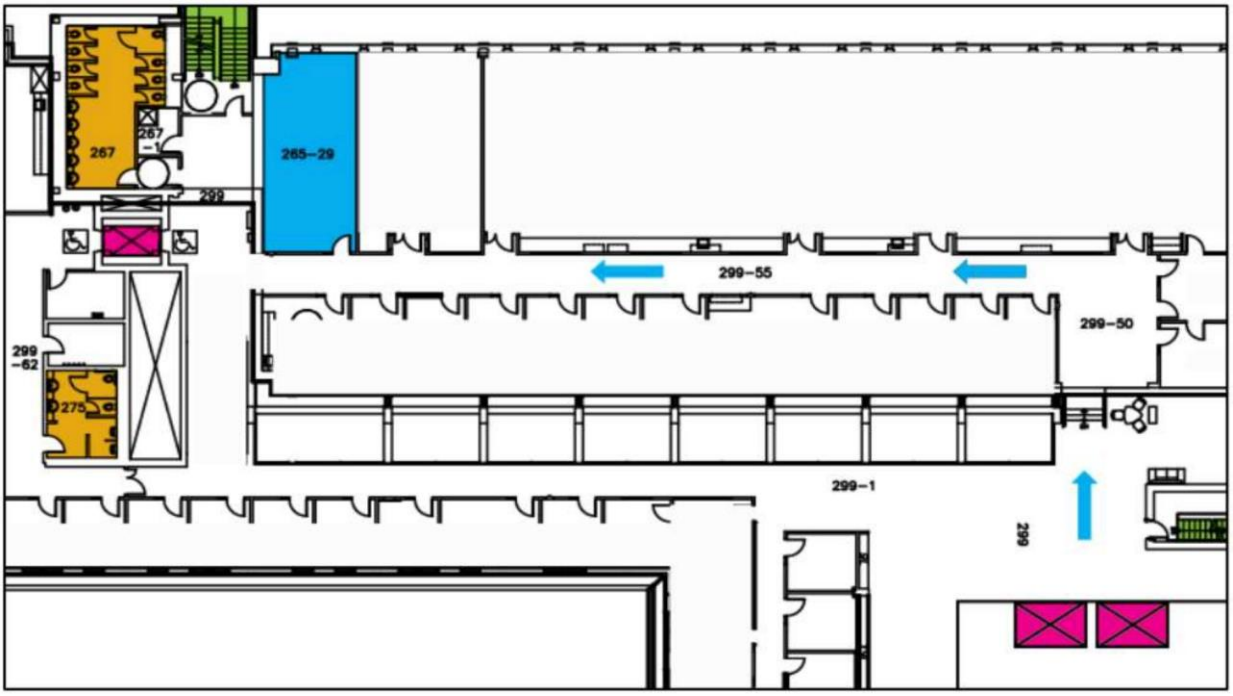

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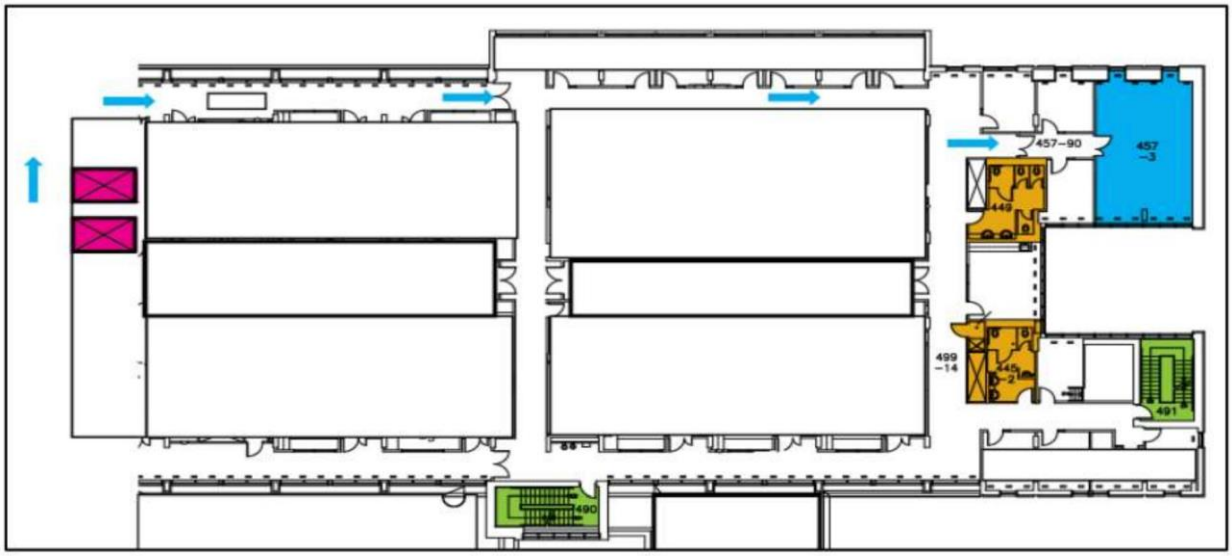
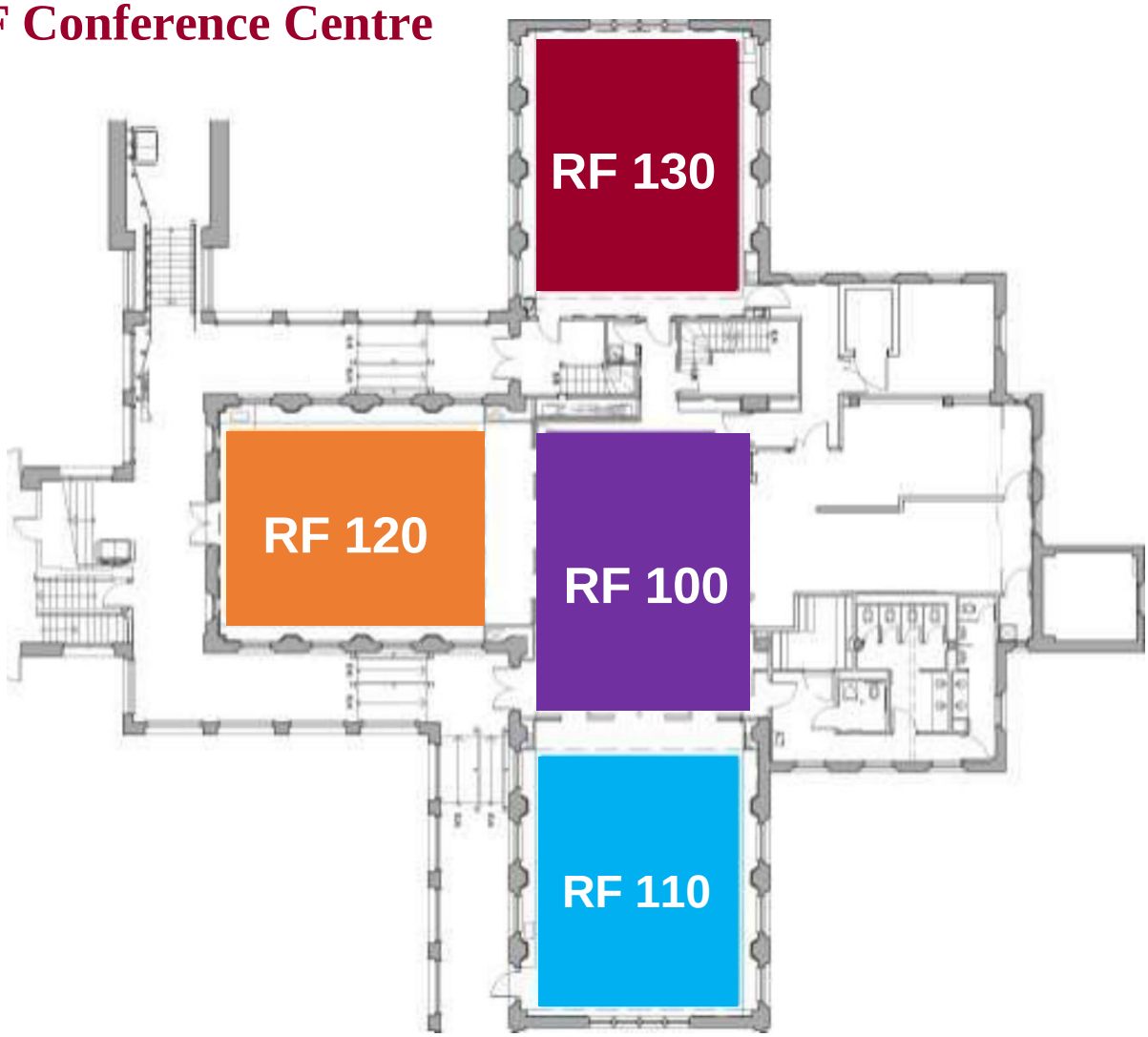


RF Conference Centre



Welcome Note // Lettre de Bienvenue

Dear friends and colleagues,

We are glad to welcome you to the 26th Annual Chemistry and Biochemistry Graduate Research Conference (CBGRC)! Two years ago, we celebrated our milestone 25th anniversary and we are excited to continue this longstanding tradition, supported by the many alumni, students, faculty, and industry professionals who have contributed to its success over the years.

The CBGRC brings together passionate researchers from across the diverse fields of chemistry and biochemistry to share ideas, innovate, and collaborate. This year, we are thrilled to host over 250 participants, including presenters, non-presenters, judges, alumni, sponsors, and our dedicated volunteers who make this event possible.

We would like to thank all participants for making the CBGRC a platform for academic and professional growth. Your unwavering dedication and enthusiasm enable this conference to thrive and expand each year.

We look forward to an engaging conference filled with inspiring discussions, innovative research, and meaningful connections. Thank you for joining us, and here’s to another successful year!

Warm regards,

The CBGRC Organizing Committee

Chers ami(e)s et collègues,

Nous sommes heureux de vous accueillir à la 26e Conférence annuelle sur la recherche des cycles supérieurs en chimie et biochimie (CBGRC)! Il y a deux ans, nous avons célébré notre 25e anniversaire et nous sommes ravis de poursuivre la tradition guidée par les nombreux anciens élèves, étudiants, professeurs et professionnels de l'industrie qui ont contribué au succès de cette conférence au fil des ans.

Le CBGRC s'efforce de rassembler des chercheurs passionnés issus des divers domaines de la chimie et de la biochimie pour partager des idées, innover et collaborer. Cette année, nous sommes ravis d'accueillir plus de 250 participants, parmi lesquels des juges, des anciens élèves, des sponsors et nos merveilleux bénévoles qui rendent tout cela possible.

Nous tenons également à remercier personnellement tous les participants pour leurs contributions visant à faire du CBGRC une plateforme de croissance académique et professionnelle en tant que chercheurs. Votre dévouement et votre enthousiasme indéfectibles sont ce qui permet à cette conférence de prospérer et de se développer année après année.

Nous attendons avec impatience une conférence engageante remplie de discussions inspirantes, de recherches révolutionnaires et de liens significatifs. Merci de nous rejoindre, et bonne année à nouveau !

Cordialement,

Le comité organisateur du CBGRC

Morning Guest Speaker (11:00 AM – 12:00 PM)

Dr. Yvan Guindon

Director, Bioorganic Chemistry Research Unit

Full IRCM Research Professor

Full Professor, Department of Chemistry, Université de Montréal

Adjunct Professor, Department of Biochemistry, Microbiology and Immunology, Faculty of Medicine, University of Ottawa

Outgoing President, RSC: The Academies of Arts, Humanities and Sciences of Canada

Member of the Board of Directors, Alberta Ingenuity Centre for Carbohydrate Science (AICCS)

Biography

Dr. Guindon is a notable figure in bioorganic chemistry, serving as Research Director at IRCM and Full Professor at Université de Montréal. His groundbreaking research focuses on synthesizing therapeutic molecules through innovative stereoselective reactions involving free radicals, with applications ranging from antiviral agents to cardioprotective compounds. Noteworthy is his development of sialyl Lewis X (sLeX) mimetics for treating conditions like sickle-cell anemia and severe lung infections, including those associated with Covid-19. With extensive experience in both academia and industry, including leadership roles in prestigious organizations like RSC: The Academies of Arts, Humanities and Sciences of Canada, Dr. Guindon's contributions have garnered international recognition, evident through his memberships in esteemed scientific societies and numerous honors, including the Order of Canada and the Queen Elizabeth II's Diamond Jubilee Medal.

Abstract: From free radical and glycochemistry to novel bioactive molecules

Our research aims to develop unique, complementary tools for synthesizing molecules that hold potential as therapeutic agents. New stereoselective methodologies involving free radical chemistry are being applied to the preparation of complex molecules such as polypropionates and all-carbon stereogenic centers. Novel families of nucleoside analogues featuring an all-carbon quaternary center at either C2' or C3' have been conceptualized, requiring the development of new synthetic methods, which are currently in progress. A series of nucleoside analogues is under study for the treatment of acute and chronic heart failure. These compounds have demonstrated cardioprotective effects across various heart failure-inducing conditions, including exposure to cardiotoxic agents, loss of survival genes, and chronic pressure overload. In addition, sialyl LewisX mimetics are being developed as E- and P-selectin antagonists for treating conditions such as vaso-occlusive crisis in sickle-cell anemia patients, cancer metastasis, severe lung infections like acute respiratory distress syndrome (a complication of Covid-19) and sepsis.

Afternoon Guest Speaker (2:30 PM – 3:30 PM)

Dr. Karine Auclair

Tier 1 Canada Research Chair in Antimicrobials and Green Enzymes

Full Professor, Department of Chemistry, McGill University

Member of the Board of Directors at Carbios

Biography

Dr. Auclair is a distinguished bioorganic chemist renowned for her groundbreaking work in combating antibiotic resistance through innovative approaches. With a focus on addressing the escalating threat of untreatable bacterial infections, Dr. Auclair's research aims to bridge the gap in antibiotic development by proposing alternative treatments that target bacteria without traditional antibiotics. By inhibiting bacterial itaconate-degrading enzymes, her work has demonstrated the ability to sensitize bacteria to natural antimicrobials produced by mammalian macrophages, leading to significant reductions in bacterial proliferation. With a prolific academic career spanning from the University of Alberta to McGill University, Dr. Auclair holds the Canada Research Chair in Antimicrobials and Green Enzymes, showcasing her expertise and leadership in the field. Through numerous awards, patents, and over a hundred peer-reviewed publications, Dr. Auclair continues to make invaluable contributions to combating antibiotic resistance on a global scale.

Abstract: Fighting bacterial infections without traditional antibiotics

Untreatable bacterial infections are expected to soon become a leading cause of death worldwide due to the increasing rate of antibiotic resistance. This is happening at a time when the development of new antibiotics has slowed dramatically, furthering the gap in the arms race between humans and bacteria. In this fight against antibiotic resistance, it is crucial to not only discover new antibiotics but also to develop alternative treatments that are less likely to select for resistance. To address this urgent problem, we propose molecules that act on bacteria, without killing them, but by making them more vulnerable to the human immune system. In particular, we have demonstrated that inhibitors of bacterial itaconate-degrading enzymes can resensitize *Salmonella* and *Mycobacteria* species to itaconate, a natural antimicrobial produced by mammalian macrophages, and lead to dramatically reduced bacterial proliferation. Since these molecules are only effective inside phagocytes and do not display antibacterial activity, they are expected to be more selective which leads to less side effects, and also show reduced frequency of resistance development.

Schedule Overview

TIME	EVENT
8:00 – 18:00	Registration (SP Atrium)
9:00 – 10:30	Student Presentations - Session A
10:30 – 11:00	Coffee Break and Sponsors Exhibition (SP Atrium)
11:00 – 12:00	Keynote Speaker 1: Dr. Yvan Guindon (GE 110)
12:00 – 13:00	Lunch and Sponsors Exhibition (RF Conference Center and SP Atrium)
13:00 – 14:15	Student Presentations - Session B
14:15 – 14:30	Coffee Break and Sponsors Exhibition (SP Atrium)
14:30 – 15:30	Keynote Speaker 2: Dr. Karine Auclair (GE 110)
15:30 – 15:45	Coffee Break and Sponsors Exhibition (SP Atrium)
15:45 – 17:00	Student Presentations - Session C
17:00 – 17:30	Coffee Break and Sponsors Exhibition (SP Atrium)
17:30 – 19:30	Poster Session (RF 110)
18:00 – 22:00	Wine and Cheese (RF Conference Center)
20:00	Award Announcements (RF Conference Center)

Student Oral Presentation Schedule

Session A // 9:00 AM – 10:30 AM

Organic Chemistry SP 157

9:10 B. D'Onofrio (*Université de Montréal*): TPDYs: Strained Macrocyclic Diynes for Bioconjugation Processes

9:25 C. Rocq (*Université du Québec à Montréal*): Asymmetric synthesis of voglibose: an anti-diabetic compound

9:40 C. Malenfant (*Université du Québec à Montréal*): Two-Step Formation of Substituted Pyridines From Iodo-Enones

9:55 C. Natola (*University of Ottawa*): Towards the Enantioselective Total Synthesis of a Novel Agro-protective Fungal Nonribosomal Peptide Synthetase—Polyketide Synthase Hybrid Secondary Metabolite

10:10 M. Denis (*Université du Québec à Montréal*): Asymmetric synthesis of gracilamine: a challenging quest

Analytical Chemistry SP 365.01

9:10 K. M. Kumaresan *(Université du Québec à Montréal):* Increasing the detectability of phosphorylated metabolites as disease biomarkers by LC-HRMS/MS

9:25 S. Matar (*Université du Québec à Montréal*): Optimized in vitro formation of sulfated metabolites and deconjugation of phase II metabolite studied by LC-HRMS/MS

9:40 D. Boivin (*Concordia University*): Selective Heart-Cutting of Low Abundance Proteins from a Capillary Array

9:55 J. Menard (*Carleton University*): Mass Spectrometry-Based Lipidomics Approach to Elucidate Biotherapeutics Production: Lentiviral Vector and Cell-Based Influenza Vaccine Production

10:10 O. Zambito (*Université du Québec à Montréal*): Multi-omic analysis of Hirschsprung disease in three mouse models by LC-MS/MS

Biochemistry & Molecular Biology RF 120

9:10 A. Clairoux (*McGill University*): Development of a capture-based method for separation of riboswitch conformational states

9:25 S. Tikoo (*Concordia University*): Synthesis of Oligonucleotide Conjugates Containing Selenium Modified Linkers

9:40 B. Albert (*McGill University*): Comparing aptamer properties for binding T cells

9:55 C. Saab (*McGill University*): Enhancing Aptamer Diversity for Targeted Therapeutics Using DNA-Encoded Libraries

10:10 C. Logan (*Concordia University*): Characterizing Probiotic Yeast Extracellular Vesicles

Inorganic Chemistry RF 130

9:25 L. Trifoi (*Concordia University*): Photon upconversion in a mixed metal cluster-based metal–organic framework

9:40 H. Bicalho (*Concordia University*): Evaluating the Photophysical Properties of a New Family of Rare-Earth Metal–Organic Frameworks

9:55 V. Lapointe (*Concordia University*): Effects of Doping on the Self-Assembly of $CsPbX_3$ Perovskite Supercrystals

10:10 C. Pomilio (*Concordia University*): Characterization of Fe-Metal Coordination Complexes for Enhanced Redox-Flow Battery Applications

Nanochemistry SP 265.29

9:10 N. Fischer (*Concordia University*): A Novel Method for Embedding Ruthenium Nanoparticles in a Metal– Organic Framework Using Direct Incipient Wetness Impregnation

9:25 P. Islas (*McGill University*): Automated Synthesis of DNA Nanostructures

9:40 M. Maia (*McGill University*): Thermo-responsive protein-polymer hybrid nanoparticles for drug delivery

9:55 C. Garcia Henao (*Concordia University*): Lanthanide-doped nanoparticles as promising persistent luminescent nanothermometers

10:10 G. Fuoco (Concordia University): Improving Carbon Dot Mediated Drug Delivery Via Drug Conjugation Through Dynamic Imine Bonds Using Mechanochemistry: A Novel Approach

Computational & Physical Chemistry SP 457.03

9:40 N. Jodaeeasl (*Concordia University*): Computational Investigation of Water-Stable Metal-Organic Frameworks for Efficient Small-Toxic-Molecule Adsorption

9:55 T. Fatoki (Federal University Oye-Ekiti): In Silico Molecular Targets, Docking, Dynamics Simulation and Physiologically Based Pharmacokinetics Modeling of Oritavancin

10:10 S. Norouzi (*Concordia University*): Docking-based screening and analysis of Bisphenol A/F/S analogs with potential endocrine disrupting activity the human estrogen receptor alpha (hERα)

Session B // 1:00 PM – 2:30 PM

Organic Chemistry SP 157

13:00 D. Patel (*Brock University*): Synthesis and Mechanistic Study of Substituted 1,2-bisphenylhydrazones: An Unintended Discovery

13:15 E. Guillet (*Université du Québec à Montréal*): Synthesis of functionalized scaffolds from phenols

13:30 G. Zorn (*McGill University*): Using Small Dipeptide Molecules to Explore Driving Forces of Liquid-Liquid Phase Separation

13:45 G. Roland (*Université de Montréal*): [2+2] Photocycloadditions to Form Cyclobutanes and Bicyclo[2.1.1]hexanes Employing Copper-Based Photocatalysis

Chemical Engineering & Environmental SP 365.01

13:00 I. S. MIR (*Université Laval*): Enhanced Fouling Resistance in Bio-Effluents Management Using Bacterial Cellulose-Graphene Oxide Composite Membranes.

13:15 J. D. Chiong (*Concordia University*): Titania Nanotube Semiconductor Arrays for Copper(I)-Bis(diimine) Sensitized Photoelectrodes

13:30 A. Niasse (*Université du Québec à Montréal*): Mécanismes De Séquestration Et Effets Toxiques Des Ions Métalliques Du Platine Et Du Palladium Chez L'algue Verte Unicellulaire Chlamydomonas ReinhardtII

13:45 R. Djidja (*Université du Québec à Montréal*): Effet de la présence de métaux sur l'ozonation catalytique de l'antibiotique Norfloxacine et son impact écotoxicologique

14:00 D. Dimitri Ruud Brelon (*Université du Québec à Montréal*): Effet du vieillissement sur les propriétés de surfaces des microplastiques: comparaison de différentes méthodes utilisées pour simuler les microplastiques environnementaux

Biochemistry & Molecular Biology RF 120

13:00 L. Domínguez Mercado (*Concordia University*): De novo resistance to “evolution-proof” Oct-TriA1 in E. coli BW25113

13:15 E. Hudson (*University of Toronto*): Synthesis of Fluorogenic Substrates for Gliomas

13:30 F. Fungo (*McGill University*): Unravelling the role of lipid peroxidation in bacterial membrane vesicle formation via fluorescence microscopy

13:45 H. Nizal (*McGill University*): Unveiling the Kinetic Tango: Exploring G-quadruplex Ligand Binding Dynamics and Transfer Mechanisms for Enhanced Therapeutic Strategies

14:00 A. Sandeep (*Université du Québec à Montréal*): Unveiling the interaction of cationic antimicrobial peptides with gram-positive bacterial cell walls

14:15 J. Arciszewski (*McGill University*): Enzymatic PET depolymerization without bulk water: a novel approach to plastic recycling

Biochemistry & Molecular Biology RF 130

13:00 N. Letourneau (*Concordia University*): Developing an anillin inhibitor for the treatment of liver cancer

13:15 S. Ouadhi (*Concordia University*): Engineering the biosynthesis of natural glycosylated natural products

13:30 I. R. Lopez-Miranda (*University of Toronto*): Development of a Long-Wavelength Photocaged β-Lapachone for Enhanced Tumor Penetration and Activation

13:45 F. R. Chowdhury (*Concordia University*): Reversing resistance using sequential antibiotic therapy

14:00 M. Thornbury (*Concordia University*): Optimizing Acid Tolerance in Kluyveromyces marxianus for Bioproduction through CRISPR-AID Screening

14:15 M. Simoes (*Concordia University*): Stress-Induced Natural Product Biosynthesis

Nanochemistry & Inorganic Chemistry SP 265.29

13:00 S. Soha (Toronto Metropolitan University): Silver-Enhanced Fluorescence: A New Frontier to Revolutionize Cellular Imaging

13:15 M. Ayachit (Queen's University): Advancements in PMMA Nanoparticle Synthesis for Drug Delivery Applications

13:30 M. A. Belahouane (*McGill University*): Zinc-Mediated Short Peptide Coacervate Microreactors for the Catalytic Breakdown of Polysaccharides

13:45 G. Turner (*Université de Montréal*): AMOX-cobalt(III) photosensitizers: promoting emission in 3d metals through charge transfers

14:00 C. Copeman (*Concordia University*): Metal–Organic Frameworks for the Adsorptive Removal of Oxyanions in Nuclear Power Plants

14:15 M. Cardoso (*Université de Montréal*): Zirconium-Based Catalysts for Stereoselective Polymerization of Polylactic Acid

Computational & Physical Chemistry SP 457.03

13:00 R. Sulaimon (*Concordia University*): Influence of Cholesterol on the Permeation of Small Hydrophobic Gases through Lipid Membranes: Insights from Molecular Dynamics Simulations

13:15 S. Mauries (*Université du Québec à Montréal*): Unusual Photochemistry in Aromatic Dithioimides: Quantitative Thione Reduction Promoted by Ether Solvents

13:30 T. Perodeau (*Université de Montréal*): Towards a better understanding of the polymer – salt coordination phenomenon in solid polymer electrolyte

Session C // 3:45 PM – 5:00 PM

Organic Chemistry SP 157

15:45 D. Farajat (*McGill University*): Nickel-Catalyzed Cross-Coupling Methylation of Aryl and Heteroaryl Electrophiles via Hydrazone Umpolung

16:00 N. Beaucage (*Université de Montréal*): Tuning Co-operative Energy Transfer in Copper(I) Complexes Using Two-Photon Absorbing Diimine-Based Ligand Sensitizers

16:15 Z. Dai (*McGill University*): Organocatalytic Peptide Coacervates as Microreactors for the Aldol Reaction in Water

16:30 K. Lebair (*Université de Montréal*): Photocatalyzed Cross-[2+2]-Cycloadditions for the Synthesis of Cyclobutanes Promoted by a Transient Copper Chromophore

Analytical Chemistry SP 365.01

15:45 E. Burovaia (*Concordia University*): LC-MS separation of 3,5-dihydroxybenzoic acid (DHBA) and 3,5-dihydroxyphenylpropionic acid (DHPPA) in human urine for nutritional studies

16:00 J. Kache Signe (*Concordia University*): Lipidomic analysis of aorta tissue reveals increased levels of phosphatidylethanolamines and phosphatidylcholines during early stages of atherosclerosis

16:15 N. Ghafari (*Université du Québec à Montréal*): Metabolomics study of polycystic ovary syndrome (PCOS) in a mouse model by LC-MS

16:30 J. McLaughlin (*Concordia University*): LC-MS Assay of NO2-Fatty Acids in Human Plasma

Biochemistry & Molecular Biology RF 120

15:45 J. Khalifa (*Université du Québec à Montréal*): Modulation of amyloid aggregation and associated toxicity with polyphenolic gallotannins

16:00 J. Ma (*University of Ottawa*): Exploiting Cytochrome P450 Promiscuity through the Chemoenzymatic Synthesis of Bicyclic Seongsanamide B

16:15 L. S. Yamout (*McGill University*): One Assay to Read-through all: a new high-resolution, high-throughput nucleic acid polymerase read-through assay

16:30 M. Mehranfar (*Concordia University*): Deciphering the regulatory role of TANGO2 in CoA metabolism

16:45 M. Boulter (*Carleton University*): Using Oriented Peptide Array Libraries (OPAL) to Identify Novel Binding Peptides for Dual Lysine and N-terminal Methyltransferase METTL13

17:00 S. Hamroff (*McGill University*): Designing the first liquid-liquid phase separating short peptides that evade irreversible amyloid-like fiber formation

Biochemistry & Molecular Biology RF 130

15:45 R. Carter (*Carleton University*): Expression profiles of modified histones suggest efficient epigenetic control in hibernating ground squirrels

16:00 C. Zhang (*McGill University*): Effects of flanking regions on DNA i-motif folding and stability

16:15 T. Ghosh (*Concordia University*): Developing Enzyme Cascades and Cell-free Strategies for Protein Engineering

16:30 Y. Wu (*McGill University*): Self-assembly of Nanostructures via the Hydrophobic Effect and DNA Base Pairing

16:45 Y. Xia (*McGill University*): Mechano-enzymatic depolymerization of highly crystalline polyethylene naphthalate under moist-solid conditions

17:00 E. T. Ali (*Concordia University*): Co-cultivation of *Aspergillus terreus* and *Myxococcus xanthus* induces the production of antimicrobial compounds in *Aspergillus terreus*

Polymer Chemistry

SP 265.29

15:45 A. Parihar (*McGill University*): Uncovering the Properties of dPGA: A Stable Alternative for Long-Term Neural Cell Culture Substrates

16:00 A. Thinphang-nga (*Concordia University*): Self-Healing Poly(Hindered Urea) Polymer Network as Coating Layer on Carbon/Sulfur Composite in High-Performance Lithium-Sulfur Batteries

16:15 K. Kadambari (*Concordia University*): Conjugated Benzoic Imine-Based Dual Acid/Light-Responsive Polymeric Nanocarriers for Enhanced Drug Delivery: Synthesis and Degradation

16:30 M. Goulet (*Université de Montréal*): Local characterization of phases in 3D-printed semi-crystalline polymers

16:45 R. Zidani (*Université de Montréal*): Preparation and characterization of polymer:photosensitizer blends

Student Poster Presentations

Poster Session // 5:30 PM – 7:30 PM

Analytical Chemistry

A01 A. Orotomah (*Concordia University*): Optimizing Protocols for Combining Imaging Mass Spectrometry (IMS) and Optical Imaging of Traditional Histologically Stained Tissues; A Step Towards Integrating IMS into Digital Pathology

A02 K. Chabi (*Université du Québec à Montréal*): Screening of Reactive Metabolites by LC-MS/MS Using Different Trapping Agents and Isotopic Labeling

Inorganic Chemistry

I01 A. MacKay (*Concordia University*): Hydroxylamines and Copper: Enabling Selective Redox Reactions *via* Ligand Design

I02 A. Saha (*Université de Montréal*): Co(III) amidine-N-oxide complexes exhibiting novel photophysical characteristics and relaxation pathways

I03 E. Lamothe (*Université de Montréal*): Synthesis and characterization of AMidine OXide (AMOX) ligands with photoactive anthracene core and their associated Ni(II) complexes photosensitizers to replace precious metal complexes

I04 H. Rammal (*Concordia University*): Controlled Synthesis of Novel Twinned MOF-199 via Reaction-Diffusion Framework In Hydrogel

I05 I. Oubaha (*Université de Montréal*): First row transition metal complexes as affordable and abundant

I06 J. F. Ricardo-Noordberg (*Concordia University*): Molecular Copper(I)-Sensitized Photoanodes for Alcohol Oxidation under Ambient Conditions

I07 T. Kourank Beheshti (*Concordia University*): Mechanochemical Synthesis of Aminoquinones

I08 T. Tesfu Abebe (*Concordia University*): Non-Random Chiral Crystallization of Epsomite

I09: E. Frappier (*Université de Montréal*): Use of redox mediator metal complexes in Chan-Evan-Lam

Physical Chemistry

Ph01 G. Amato (*Concordia University*): Chiral Induced Spin Selectivity in Triboelectric Nanogenerators

Ph02 Y. Li (*Queen's University*): An investigation of CO_2 laser pattern creation on Polydimethylsiloxane thin film surface in daytime passive radiative cooling

Ph03 M. Lormahdiabadi (*Université de Montréal*): Impact of Antibacterial Cysteine-Derived Carbon Dots on the Biophysical Properties of Pulmonary Surfactant

Organic Chemistry

O01 A. McAlpine (*McGill University*): Pantothenamide-mimicking compounds as novel antimicrobial agents

O02 H. Braga (*Concordia University*): Drug Design, Synthesis and Structure-Activity-Relationship Studies of 1,3,5-Triazine Derivatives as Positive Allosteric Modulators for G-Protein-Coupled Receptor 68 (GPR-68)

O03 S. Taylor (*Concordia University*): The Development of Anillin-Specific Inhibitors for Treatment Against Hepatocellular Carcinoma

O04 K. Burchell-Reyes (*Laval University*): Synthesis and enantioselective reduction of prochiral α- CF_3 and α-SF_5 ketones

O05 O. Ortiz (*Polytechnique Montréal*): Photostable Open-Shelled Fluorophores For Near-Infrared Organic Light-Emitting Diodes: A Proof Of Concept

O06 R. Lessard (*Université de Sherbrooke*): Influence of Fluorine on Sterically Controlled Rhenium-catalyzed Hydroxyl Transposition to Access Enantioenriched Quaternary Centers.

Molecular Biology

M01 J. De la Garza (*Concordia University*): Uncovering the Protein Sorting Machinery of the Intralumenal Fragment Pathway for Membrane Remodelling

M02 K. Hon (*Concordia University*): An Automated Approach to Streamline EV tag Discovery in Yeast.

M03 S. Rehman (*Carleton University*): Small RNA and Freeze Survival: The Cryoprotective Functions of MicroRNA in the Frozen Muscle Tissue of The Grey Tree Frog

M04 I. Rhzali (*Carleton University*): Histone Arginine Methylation in the Wood Frog, Rana sylvatica

M05 J. Trani (*Concordia University*): Expressing the human proteome in Saccharomyces cerevisiae as a model for advancing extracellular vesicle biology

Environmental Chemistry

E01 T. Cha-Cossette (*Université du Québec à Montréal*): Lithium recovery characterization with Ion sieve material

E02 C. Johannessen (*Concordia University*): From Properties to Impacts: Environmental Modeling of Tire-Derived Chemicals

E03 M. Ezzati(*Concordia University*): A Methodological Investigation into the Analysis of Organic Matter Linked to Iron Oxides in Marine Sediments

Biochemistry

B01 A. Ahaffai (*Université du Québec à Montréal*) : Impact de la SUMOylation sur les interactions de MeCP2 : Vers de nouvelles perspectives thérapeutiques pour le syndrome de Rett

B02 J. Bennett (*McGill University*): Reprogramming DNA with a Small Molecule

B03 A. Chang (*McGill University*): Investigating the enzymes of a novel pathway to treat bacterial infections

B04 J. Enright (*Carleton University*): Investigating the Efficacy of Novel Peptides in combination with β-lactam antibiotics against the TEM1 β-lactamase

B05 V. Ezeduru (*McGill University*): Defining the functional properties of cyclopropane fatty acid synthase from Pseudomonas aeruginosa

B06 G. Hanna (*McGill University*): Unraveling Lanthipeptide Biosynthesis: High-Resolution Insights via Nuclear Magnetic Resonance.

B07 M. Khammar (*University of Sherbrooke*): Assembly of MacAB-TolC, a multidrug efflux pump, and its role in antimicrobial resistance

B08 E. Khanjani (*Concordia University*): An enzymatic pathway for [18F] FDG synthesis on a microfluidic platform.

B09 H. W. Petit-Frère (*Université du Québec à Montréal*) : Étude de l'importance des motifs d'interaction à SUMO (SIMs) dans le mécanisme de SUMOylation et leur utilisation pour la conception de nouvelles SUMO E3 ligases synthétiques pour des applications biotechnologiques.

B10 B. Pattanayak (*IRCM, McGill University*): Characterisation of the interactome of Cytohesins, a family of ARF-GEFs, in ARF signaling and in the regulation of focal adhesions.

B11 S. Qin (*McGill University*): Capturing the Conformational Dynamics that Define Lanthipeptide Synthetase Enzymatic Function using Single Molecule Fluorescence Spectroscopy

B12 T. Rutherford (*Concordia University*): Synthesis and Characterization of DNA Tetrahedra Containing O6- Alkylene 2'-Deoxyguanosine Cross-Links for Controlled Disassembly Triggered by a DNA Repair Protein

B13 J. F. Sanchez Tejeda (*McGill University*): Synergizing Photosensitizers and LDE Metabolism with Ferroptosis for Targeted Cell Death

B14 R. Wang (*Carleton University*): Investigating SMYD3 Oncogenic Activity by Machine Learning: Discovering Novel Substrates and Peptide-Based Inhibitors

Computational Chemistry

C01 J. Genzling (*McGill University*): From Organic Principles to Predictive Models: Advancing pKa and Geometry Calculations with Graph Neural Networks

Nanochemistry

N01 D. Ali (*Concordia University*): Phytoglycogen nanoparticles: a promising nanocarrier for the inhalation delivery of antibiotics

N02 A. Clermont-Paquette (*Concordia University*): Fluorescent carbon dots: A novel bioimaging tool to reveal the mechanism of action of anticancer drugs in cells

N03 T. Das (*McGill University*): Characterizing the cellular interaction of DNA nanostructures from *in-vitro* to *in-vivo*

N04 F. Gamez (*McGill University*): Development of optical biosensor based on GQD/ZnO for potential detection of *Salmonella typhi*

N05 C. Guérin (*Université de Montréal*): Gold-Supported Lipid Membranes Formed by Redox-Triggered Fusion: A Study of The Thermotropic Properties

N06 V. Passos Gibson (*CHUSJ*): Layer-by-Layer-modified lipid nanoparticles for miR-181a delivery in glioblastoma treatment

N07 M. Paziresh (*Queen's University*): The formation of nanodendritic silver structures from a silver salt solution via continuous-wave laser irradiation

Chemical Engineering

E03 J. Wu (*Concordia University*): Towards BioFoundry on a Chip – A Digital Microfluidic Platform for DNA Synthesis by Phosphoramidite Chemistry

Polymer Chemistry

P01 M. Wolff (*McGill University*): Scaling Carboxylated Cellulose Nanocrystals to Make Functional Microspheres

P02 U. Mody (*The University of British Columbia*): Photo initiator and Acrylate Free Photo-cross linkable Hydrogel

ANALYTICAL CHEMISTRY

Heart-Cutting for Low Abundance Proteins from a Capillary Electrophoresis Array

D. Boivin[1*], C. Skinner[1]
Concordia University

Proteoform profiling, the identification of variant permutations of a single protein species is of immense interest to the clinical, biotherapeutic and academic fields. The sub-classification of a single protein isotype (a unique amino acid sequence) is a required critical quality attribute (CQA) to assess the safety of some biotherapeutic drugs. Large, highly conserved proteins, with subtle post translational modifications (PTM) such as monoclonal antibodies (mAbs), pose a significant challenge for separation and proteoform identification. Capillary electrophoresis (CE) is, to date, the only electrophoretic method capable of performing native mAbs separation, a requirement for deep proteoform profiling. Here we propose to use a series of 5 parallel CE separations, each of increasing length, to carry-out the initial high resolution protein separation. The CE effluent(s) are released in a custom-built heart-cutting sheath-flow-interface (SFI) where a repositionable capture capillary is used to capture the same isoform peak from the 5 capillaries. The key advantages of this approach are the initial high-resolution separation, an exchange into buffer/solvents more suited to proteoform profiling upon capture, and numbering-up by using multiple parallel separations. These advantages will be demonstrated by isolating minor mAb variants that will be assesses for purity, AIS and profiled to identify the PTMs.

LC-MS separation of 3,5-dihydroxybenzoic acid (DHBA) and 3,5- dihydroxyphenylpropionic acid (DHPPA) in human urine for nutritional studies

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Alkylresorcinols (ARs) are a class of phenolic lipids comprising of an alkyl chain of up to 27 carbon atoms attached to a resorcinol ring. ARs have been identified as biomarkers of whole grain consumption. In the human body, ARs are metabolized through β-oxidation, resulting in the production of 3,5-dihydroxybenzoic acid (DHBA) and 3,5-dihydroxyphenylpropionic acid (DHPPA).The objective of this study was to develop a novel liquid chromatography–tandem mass spectrometry (LC-MS) method for accurate and precise measurement of DHBA and DHPPA in human urine. Assay development entailed the optimization of electrospray ionization parameters, LC separation, and extraction methodologies. We conducted a comparison of different types of stationary phases, including biphenyl, silica, HILIC-Z, and mixed mode, with the objective of determining the LC parameters that would provide the best separation. Particular attention was paid to the separation of known isomers of both analytes of interest. Furthermore, the impact of varying the strength of the injection solvent was examined for the most promising LC separations to ensure adequate analyte solubility while maintaining good peak shape. For HILIC methods, 70-90% acetonitrile was suitable for DHPPA, while for DHBA, the optimal results were obtained with 70% acetonitrile.

Metabolomics study of polycystic ovary syndrome (PCOS) in a mouse model by LC-MS

N. Ghafari[*], S. Nawaito, O. Souchkova, N. Pilon, L. Sleno
Université du Québec à Montréal

Polycystic ovary syndrome (PCOS) is a common hormonal disorder affecting 8-13% of women. The condition is characterized by a hormonal imbalance resulting in many symptoms, including infertility, acne, excessive hair growth and weight gain. The causes of the disease are still unknown, and no cure has yet been found.

The aim of this project is to study the metabolic variations caused by polycystic ovary syndrome, and the impact of a metformin/bile acid combination therapy. To this end, a liquid chromatography-tandem mass spectrometry (LC-MS/MS) metabolomics study was carried out using plasma and feces sample from PCOS model mice. Metabolites were extracted from three sample groups (healthy, disease and treated). Targeted analysis was performed using a commercial kit to quantify 546 molecules in plasma samples. A non-targeted approach was also adopted to complement these results, with over 347 and 198 metabolites identified in feces and plasma samples, respectively. The results obtained with this exploratory approach enabled us to recognize specific metabolic pathways disrupted by PCOS in this mouse model, as well as the impact of treatment on these perturbations.

Lipidomic analysis of aorta tissue reveals increased levels of phosphatidylethanolamines and phosphatidylcholines during early stages of atherosclerosis

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Concordia University

Atherosclerosis is the major cause of cardiovascular diseases. Western (W) and low-carbohydrate-high- protein (L) diets are atherogenic in apolipoprotein-E knocked-out (ApoE-ko) mice, and the lipid characterisation of vascular tissue can provide novel insights how the two diets contribute to atherogenesis.

This study aimed to investigate the lipid profiles of the aorta tissues of ApoE-ko mice fed a W or a L diets compared to the normal-chow (C) diet.

Male ApoE-ko mice were randomized into three groups: W-group, L-group and C-group (n = 12 each). After 6 weeks, aorta samples were collected and homogenized, lipids extracted with isopropanol, and lipid profiles measured using untargeted lipidomics workflow combining C18 liquid chromatography and Orbitrap MS with data-dependent acquisition. LipidSearch 5.0 was used to annotate lipids.

Principal component analysis indicated a clear difference between the lipid profiles of mice fed C diet versus pathology groups. Mice fed L or W diets showed similar lipid dysregulation, with several phosphatidylethanolamines (PEs) and phosphatidylcholines (PCs) showing significant increases in the W and L-groups. PEs and PCs are implicated in the regulation of inflammation.

These findings provide new insights into lipid dysregulation in the vascular tissue of mice during initial stages of atherosclerosis.

Increasing the detectability of phosphorylated metabolites as disease biomarkers by LC-HRMS/MS

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Metabolites are small biomolecule products and intermediates of metabolism that drive reactions that are essential for the survival of an organism. Phosphorylated metabolites are known to play essential roles in metabolic pathways such as glycolysis, the pentose phosphate pathway and lipid metabolism. Due to their role in various metabolic pathways, perturbations in phosphometabolite concentrations can be linked to energy-related disorders. However, in many cases, phosphorylated metabolites are hard to detect and analyse in complex biological samples. We are developing an optimized workflow for sample preparation and increased detectability by liquid chromatography – tandem mass spectrometry (LC-MS/MS) of these phosphometabolites. This presentation will show an overview of our results in various biological sample types in the context of studying disease models.

Optimized *in vitro* formation of sulfated metabolites and deconjugation of phase II metabolite studied by LC-HRMS/MS

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We have tested different conditions for the formation of sulfated metabolites of various xenobiotics using *in vitro* incubations, with subsequent characterization of these metabolites by liquid chromatography coupled to high-resolution tandem mass spectrometry. These incubations were conducted with liver S9 fractions using two distinct cofactors: ATP or PAPS, the latter being unstable and very costly. Results showed that ATP and inorganic sulfate effectively produced sulfated metabolites, suggesting a less expensive alternative to PAPS for compound sulfation, as well as improved metabolite detection due to the regeneration of PAPS in vitro using this system.

Following this, a method was developed to test enzymatic deconjugation conditions for glucuronidated and sulfated metabolites formed in vitro and present in urine sample, to transform phase II metabolites for simplified detection of their unconjugated precursors. This presentation will discuss this approach and its usefulness for untargeted exposomics analysis in biological fluids.

LC-MS Assay of NO_2-Fatty Acids in Human Plasma

J. McLaughlin*, L. C. Cougnaud, D. Vuckovic
Concordia University

Nitro-modified fatty acids (NO_2-FAs) are a class of bioactive, unsaturated lipids involved in various biological processes, including inflammatory response, oxidative stress, and cell proliferation. They are also currently under investigation as therapeutic agents. Oxylipins are a related class of lipids, also composed of an unsaturated fatty acid but modified with oxygen species, with similar biological roles. Although various LC-MS based methods for oxylipins currently exist, NO_2-FAs and their derivatives remain understudied. The objective of this study was to develop LC-HRMS method for the simultaneous analysis of oxylipins and NO_2-FAs. This method combines C18 SPE with reversed-phase C18 LC-HRMS on Q-ToF. This method has been used to separate more than 70 oxylipins and several putative NO_2-FAs in murine and human plasma. In standards, the method was able to separate key currently known isomers of NO_2-FAs. Extraction recovery ranged from 71-83% across the range of oxylipins tested. Matrix effects were also evaluated and ranged from 87-98%, indicating no significant ionization effects. In conclusion, this method capitalizes on high resolution profiling to enable simultaneous analysis of both classes of compounds, thus opening up new avenues to study NO_2-FAs.

Mass Spectrometry-Based Lipidomics Approach to Elucidate Biotherapeutics Production: Lentiviral Vector and Cell-Based Influenza Vaccine Production

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With the advancements of novel biotherapeutics, such as lentiviral vector (LV) gene therapies and cell-based influenza vaccines (CIVs), significant efforts to ameliorate biomanufacturing pipelines are being made to make these therapeutics as cost-effective as possible. With lipids being critical components of cells and viruses, it is essential to understand the lipidomic dynamics of producing cells and viroceutical products. We developed a rapid, robust, and sensitive untargeted liquid chromatography-mass spectrometry (LC-MS) lipidomics pipeline to analyze novel biotherapeutic products and demonstrate its utility in producing cells and the final viral product. For LV production, HEK 293T-producing cells were severely depleted in phospholipids, while storage lipids significantly increased, signifying critical lipidomic dynamics in response to virus production. The characterization of the final LV product provides a potential list of lipids for quality control metrics during the biomanufacturing process. For CIV production, the heterogeneity of MDCK cell clones lead to distinct lipidomics profile, virus production dynamics, and a unique influenza viral envelope profile. Our approach can be readily used to study the lipid dynamics of large-scale biotherapeutics production, be rapidly translated into targeted methods to quantify individual lipid components and offer insights to improve upstream biomanufacturing of biotherapeutics.

Multi-omic analysis of Hirschsprung disease in three mouse models by LC-MS/MS

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Hirschsprung disease is a rare disease characterized by the absence of nerve cells in the distal region of the colon, leading to severe functional obstruction. This disease, which affects approximately 1/5000 live births, is more common in boys (4x) and newborns with Down syndrome (100x). Affected children develop dangerous infections leading to major complications, including death.

To better understand disease pathogenesis, three genetically distinct mouse models, *Holstein* (modeling the association with Down syndrome), *TashT* (modeling the male bias) and *Piebald-Lethal* (modeling the association with EDNRB mutations), were studied with the aim of distinguishing changes in protein and metabolite levels in colon tissue and feces samples. Samples collected from the proximal and distal regions of the colon were used for untargeted metabolomics and proteomics analyses using liquid chromatography coupled with high-resolution tandem mass spectrometry. We will present the methodology developed for the quantitative multi-omics approach, as well as the results of this study and the perspectives for future work.

Evaluating the Photophysical Properties of a New Family of Rare-Earth Metal–Organic Frameworks

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Nearly thirty years after the first use of the name metal–organic framework (MOF), this class of materials is receiving more attention than ever, being considered by many as the future of materials science. These distinguished materials are composed of metal ions or clusters bonded by organic linkers, giving rise to three- dimensional network structures. Because of their very interesting characteristics, which often include extensive porosity, crystallinity, and structural tunability through controlling the inorganic and organic building units, more than 100,000 different MOFs have so far been reported.

Due to the special characteristics of rare-earth (RE) elements, which include scandium, yttrium, and the whole lanthanoid series, promising new RE-based MOFs have been obtained in the past years. Among these characteristics, it is worth mentioning the high coordination numbers and distinct optical properties of RE ions, which can lead to the generation of materials with interesting photophysical and photochemical properties and unique crystalline structures.

In this work, a series of RE-MOFs based on the archetypical zirconium MOF-808 were obtained through a *de novo* synthetic approach. A series of studies were carried out in order to optimize the synthetic conditions and the final materials were fully characterized and studied regarding their photophysical properties.

Metal–Organic Frameworks for the Adsorptive Removal of Oxyanions in Nuclear Power Plants

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Nuclear power represents 10% of global electricity production, and 28% of low carbon electricity generation. To keep power plants running safely and efficiently, the water used must be ultrapure, to prevent corrosion or interference in the nuclear reaction. Oxyanions of various elements are common contaminants in water used in the generation of electricity at nuclear power plants. 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 $\eta_2\mu_2$ fashion. Herein, adsorption of oxyanions on Zr_6-based MOFs will be discussed, including the kinetics of adsorption, maximum uptake capacity, and characterization of the adsorption mechanism as well as the effect of harsh conditions present in power generation environments on the MOF adsorption characteristics and material stability.

Effects of Doping on the Self-Assembly of $CsPbX_3$ Perovskite Supercrystals

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Concordia University

Supercrystal formation afforded by the self-assembly of cesium lead halide ($CsPbX_3$) perovskite nanocrystals has been a phenomenon of interest due to the high three-dimensional structural order required and the resulting properties. The high structural order is influenced by the surface chemistry and particle morphology
of the starting nanocrystal building blocks. Ion doping into metal halide perovskite nanocrystals has also been investigated as these dopants have been found to improve their optoelectronic and morphological properties while also imparting other characteristics not originally present in the metal halide perovskites. In this work, we investigate the structural and photophysical effects of dopants on cesium lead halide perovskite supercrystals through absorbance and photoluminescence spectroscopies, photoluminescence quantum yields, powder X-ray diffraction, and electron microscopy.

Characterization of Fe-Metal Coordination Complexes for Enhanced Redox-Flow Battery Applications

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Concordia University

The world is in need of reliable and renewable energy alternatives to fossil fuels. However, since most renewable energies do not supply continuous power, it is important to have clean energy storage methods. Electrochemical energy storage technologies such as redox-flow batteries are of interest because they offer a cheap and sustainable energy source option. Redox-flow batteries are comprised of multiple components, such as electrolyte solutions, half-cells, a membrane, electrodes, pumps, and a power source. Of particular focus are the chemical components responsible for the redox activity in the battery. To date, various electrolyte solutions composed of metal-ligand coordination complexes dissolved in salt solutions, have been explored. However, the key is that the electrolytes must be electrochemically compatible in order to be employed together in the battery. Herein, we investigate the synthesis and characterization of iron 2+/3+ ethylenediaminetetraacetic acid complexes and iron 2+/3+ 2,2'-bipyridine complexes, as electrolytes in redox-flow batteries. Preliminary characterization and evaluation of these iron-based complexes include infrared and optical spectroscopies, optical microscopy, Pourbaix analyses, ground state electrochemistry and battery cell cycling.

Photon upconversion in a mixed metal cluster-based metal–organic framework

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Upconversion is a non-linear optical process involving the absorption of two or more low-energy photons, converted and emitted as higher-energy photons. Lanthanide-based upconverting nanoparticles **(Ln-UCNP)** exploit the unique energy level configurations and energy transitions of trivalent lanthanoid ions, and offer promising applications in fields such as optoelectronics, energy harvesting and biomedicine. In the past decade, metal–organic frameworks (MOFs) have garnered tremendous interest owing to their remarkable structural diversity and chemical tunability. Although MOFs have applications in numerous fields, their use as upconverting materials remains widely unexplored. This study explores the integration of lanthanoid activators and sensitizers within cluster-based RE-UiO-66 MOFs, demonstrating their synthesis, optical properties, and upconversion mechanisms. Our findings unveil the first instance of upconversion in cluster- based MOFs, suggesting new pathways for integrated activator-sensitizer MOF systems in advanced photonic applications.

AMOX-cobalt(III) photosensitizers: promoting emission in 3*d* metals through charge transfers

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Developing alternative fuel sources fuels is an important challenge of the 21st century. Artificial photosynthesis can help us reach this goal, but its use needs to be sustainable. Luckily, many developments have occurred in the last fifteen years with first-row metal-based photosensitizers. This project joins in the search, bringing in new cobalt(III) complexes based on aminine N-oxide (AMOX) ligands. These ligands' strong sigma donation destabilizes MC excited states responsible for much of 3*d* metals' non-radiative decay. Additionally, the AMOX ligands designed in this work possess sufficient conjugation to stabilize its mixed metal-ligand frontier orbitals. The HOMO-LUMO transition thus becomes a mixed LMCT, and its corresponding excited state is even more stable than any MC stattes it has. This eliminates an important source of non-radiative quenching, leading to nanosecond-order excited state lifetimes.

Unusual Photochemistry in Aromatic Dithioimides: Quantitative Thione Reduction Promoted by Ether Solvents.

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We report a mechanistic investigation of an aromatic dithioimide (**2SS**) displaying puzzling yet efficient photochemistry in ether solvents. Perplexingly, **2SS** dissolved in ether solvents in a sealed and degassed vial was photochemically converted to the corresponding diimide (**2OO**), as determined by ^{1}H NMR following product extraction. With no external sources of oxygen in the sample, could the oxygen in **2OO** be from the ether itself? To study this unprecedented proposition, we attempt to uncover the ether's involvement in this reaction. As seen by laser-flash photolysis, **2SS** appears to first react with the solvent from its singlet excited state. Following the reaction by NMR under rigorously oxygen- and water-free conditions led to the identification of a photoreductive pathway that quantitatively transformed one thione into a methylene to yield **2SH2**. Subsequent oxidation of **2SH$_2$** or irradiation of **2SS** under air proved that molecular oxygen was indeed necessary to observe an oxidative pathway leading to **2OO**, ruling out the initially proposed involvement of an ether oxygen. An explanation of **2SS** desulfurization was further revealed through the study of solvent by-products by GC-MS analysis. Supported by DFT calculations, a mechanism is proposed to involve a chain reaction initiated by photochemically generated ether radical.

Towards a better understanding of the polymer – salt coordination phenomenon in solid polymer electrolyte

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The development of solid polymer electrolyte for electrochemical applications such as energy storage devices enables a safer and denser energy storage solution to the ones currently available. Fundamental understanding of ionic transport through interaction strength and polymer chain relaxation in the solid and melted states is necessary to develop better electrolytes. In this work, we developed and applied a characterization method through multiple techniques allowing us to interpret the impact of the salt coordination on the ionic transport of a solid polymer electrolyte's The polycaprolactone (PCL) / lithium bis(trifluomethane)sulfonimide (LiTFSI) system studied was analyzed by differential scanning calorimetry (DSC), variable temperature infrared spectroscopy (FT-IR), electrochemical impedance spectroscopy (EIS) and oscillatory rheology. Polyester electrolytes being less reported than their polyether counterparts, the phase diagram of the PCL / LiTFSI system was constructed from DSC results. FT-IR spectroscopy allowed to probe the coordination environment of the lithium salt as a function of concentration while temperature FT- IR enabled a quantitative evaluation of an interaction strength between the lithium cation and the carbonyl moiety of PCL. Comparative analysis of the results obtained allowed a fundamental understanding of the impact of coordination strength on ionic transport in the solid and melted states.

Tuning Co-operative Energy Transfer in Copper(I) Complexes Using Two-Photon Absorbing Diimine-Based Ligand Sensitizers

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Université de Montréal

Photocatalysis mediated by low energy light wavelengths has potential to enable safer, sustainable synthetic methods. A phenanthroline-derived ligand **bathocupSani**, with a large two-photon absorption (TPA) cross section was used to construct a heteroleptic complex [Cu(**bathocupSani**)(**DPEPhos**)]BF_4 and a homoleptic complex [Cu(**bathocupSani**)$_2$]BF_4. The ligand and the respective homoleptic complex with copper exhibit two-photon upconversion with an anti-Stokes shift of 1.2 eV using red light. The complex [Cu(**bathocupSani**)$_2$]BF_4 promoted energy transfer photocatalysis enabling oxidative dimerization of benzylic amines, sulfide oxidation, phosphine oxidation, boronic acid oxidation and atom-transfer radical addition.

Zinc-Mediated Short Peptide Coacervate Microreactors for the Catalytic Breakdown of Polysaccharides.

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McGill University

The naturally occurring polysaccharides found in nearly all plant matter represent a near limitless regenerative source of valuable carbohydrate desirable as building blocks for chemical synthesis. Yet despite much effort to synthetically emulate the efficiency at which enzymes catalyze the breakdown of these recalcitrant natural polymers for large scale production, there still lacks a desirable method that is sustainable both environmentally and economically while still efficient.
A library of short dipeptides bearing slight structural alterations when mixed with sufficient zinc chloride were found to generate exceptionally turbid solutions rich in coacervates that form via rapid liquid-liquid phase separation. These zinc coacervate phases were found to not only be stable under highly acidic conditions but also exceptionally adaptable towards a wide range of physical and chemical changes in their environment such as elevated temperatures and the presence of different metal ions. We aim to capitalize on these unique properties by designing a system of Zinc coacervates rich in modified diphenylalanine to generate liquid microreactors adept at loading small disaccharides via favorable CH- π interactions into an environment crowded with Lewis's acids to drive hydrolysis into smaller sugars.

TPDYs: Strained Macrocyclic Diynes for Bioconjugation Processes

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A terphenyl diyne (TPDY) macrocycle, 3,5-TPDY, has been developed for bioligation. The reagent incorporates a highly bent 1,3-diyne that is active in SPAAC processes affording atropoisomeric triazole products. The TPDY is also viable in cycloadditions with diazoacetates and tetrazines with complementary kinetics. The 3,5-TPDY derivative was found to be bench stable and easily accessible via a streamlined two- pot synthesis. A pendant amine allowed bioconjugation of TPDY to two proteins in a microbial transglutaminase-catalyzed reaction. The resulting TPDY-conjugated crystallizable fragment of IgG1 antibody (hFc) and B domain of protein G (GB1) were subsequently labelled with a fluorophore via SPAAC, demonstrating ease of application. Importantly, in contrast to many cycloalkyne SPAAC reagents that exploit π→σ* hyperconjugation to stabilize ground states, the TPDY stabilization occurs via interactions of π and π* orbitals of the adjacent alkynes.

Organocatalytic Peptide Coacervates as Microreactors for the Aldol Reaction in Water

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McGill University

The organocatalyzed aldol reaction in aqueous conditions has attracted considerable interest since the pioneering reports in the early to mid 2000s. However, current catalytic systems can require harsh additives, long reaction times, or challenging and expensive syntheses. Our group recently reported that short peptide sequences can form coacervate droplets in water, which can enhance reaction rates by concentrating reagents in a hydrophobic microenvironment. By attaching a proline to the peptide, we obtained organocatalytic coacervates which can serve as microreactors in water. Stabilized by the ketone reagent and a surfactant additive, these coacervates were effective in the aldol reaction in water, affording products in high yields and moderate diastereo- and enantioselectivity. This is, to our knowledge, the first example of an inherently organocatalytic coacervate, representing an easily accessible and green catalytic platform.

Asymmetric synthesis of gracilamine: a challenging quest.

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Université du Québec à Montréal

Among the many alkaloids provided by Mother Nature, the Amaryllidaceae family includes a broad variety of bioactive molecules, such as the Lycorane-type. Gracilamine, which belongs to this family, is the most complex alkaloid. It represents a considerable synthetic challenge due to its hexacyclic structure with 7 contiguous stereocenters including 2 quaternary carbon centers. Starting from **tyrosine**, **leucine** and
piperonal, three abundant natural molecules, we are on the way to produce an asymmetric total synthesis of Gracilamine. Our approach involves an oxidative phenol dearomatization mediated by a hypervalent iodine reagent, a diastereoselective aza-Michael process and a cycloaddition [2+3] with leucine developed by the Ma group.

Nickel-Catalyzed Cross-Coupling Methylation of Aryl and Heteroaryl Electrophiles via Hydrazone Umpolung

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Methyl groups play a vital role in pharmaceutical substrates, where their installation onto aryl and heteroaryl moieties can often lead to enhanced drug-target interactions. This phenomenon has been termed the “magic methyl effect”, and it has become an important tool for the improvement of therapeutic potency during lead optimization stages in drug development. Herein, we report a new methodology for the methylation of various phenols as tosylates as well as aryl halides via a hydrazone-mediated Ni-catalyzed cross-coupling by introducing a new bench-stable methylating reagent in the form of formaldehyde hydrazone. The reaction produces moderate to good yields ranging from 28-89% on a structurally diverse set of aryl and heteroaryl electrophiles. Late-stage functionalization of medicinally relevant compounds including *beta*-estradiol and ezetimibe were also achieved. Experimental and computational investigations were carried out to support the proposed mechanism for this reaction.

Synthesis of functionalized scaffolds from phenols

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The synthesis of polyfunctionalized dienones from readily available phenols is a promising tool for organic chemistry. Products are obtained through an aza-Michael addition and elimination reaction sequence, on dearomatized phenolic substrates mediated by hypervalent iodine reagents. Those molecules represent interesting precursors for the total synthesis of natural products, due to their highly versatile structure, produced from affordable starting materials. In addition, we are currently developing an asymmetric synthetic pathway for these products, involving a biocatalytic process with commercial enzymes. Thus, developing a green catalytic process enables the synthesis of asymmetric skeletons through a desymmetrization step.

Photocatalyzed Cross-[2+2]-Cycloadditions for the Synthesis of Cyclobutanes Promoted by a Transient Copper Chromophore

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These days, faced with economic and environmental challenges, the chemical industry needs to move increasingly towards greener, more responsible processes. The project is based on the use of photocatalysis as an alternative to popular processes using the noble metals ruthenium and iridium.

For this reason, copper is the metal of choice for this project. Recent examples of alkene reactivity from the Poisson and Collins groups using copper in photochemistry have brought significant and solid advances over processes carried out by its more expensive counterparts. Energy transfer reactions and single electron transfer have been very much in vogue in recent years, and are tending to become even more widespread.

This process allows access to excited states of compounds previously difficult to reach. Copper complexes are capable of carrying out these processes, highlighting the capabilities and modularity of the latter, the result of a synthesis of the latter that has become very accessible. This work highlights copper's ability to sensitize alkenes, including cinnamate derivatives, via an inner sphere process. The latter are reagents of choice for carrying out [2+2] cycloaddition reactions in the presence of various olefins. The method has enabled us to develop a wide range of polysubstituted cyclobutanes.

Two-Step Formation of Substituted Pyridines From Iodo-Enones

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A new access to substituted pyridines was developed from iodo-enones. This two-step procedure involves a Sonogashira coupling with a free alkyne containing a nosylamide followed by a thiophenol treatment in basic conditions that triggers a nosyl deprotection, a Michael-retro-Michael process, a condensation and isomerization in cascade to yield the heterocycle. This method enables the introduction of different substituents at several pyridine positions. This approach offers new synthetic opportunities to produce heterocycles present in many bioactive compounds.

Towards the Enantioselective Total Synthesis of a Novel Agro-protective Fungal Nonribosomal Peptide Synthetase—Polyketide Synthase Hybrid Secondary Metabolite.

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Fusarium head blight (FHB) is a major fungal disease impacting cereal crops in Canada, with Agriculture and Agri-Food Canada (AAFC) tracking its rise since 1995 and estimating $1 billion CAD in losses during a 2016 epidemic. In partnership with AAFC, we discovered a novel hybrid polyketide synthase-nonribosomal peptide synthetase (PKS-NRPS) secondary metabolite produced by *Fusarium avenaceum*. This metabolite has shown promising biological activity, possibly influencing the plant immune response. In this study, we describe its total synthesis to clarify its molecular structure. While 1D and 2D NMR data confirm the backbone connectivity, stereochemistry remains undetermined. Initial model studies identified a diastereoselective macrolactamization as optimal for macrocyclization between the dipeptide backbone's amino acid residues. We are also exploring an enantioselective, modular approach to construct the PKS fragment, providing access to all potential diastereomers. This flexible synthesis route supports practical manipulations to define stereochemistry. We will present the completed synthesis, focusing on its utility in structural characterization, and report bioactivity assays of intermediates to pinpoint the active pharmacophore. Our work could offer novel insights and tools for FHB control, with implications for crop protection and agricultural resilience.

Synthesis and Mechanistic Study of Substituted 1,2-bisphenylhydrazones: An Unintended Discovery

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This research investigates the synthesis of various substituted 1,2-bisphenylhydrazones. Initially, upon reacting a substituted phenylhydrazine with a keto amide to yield a hydrazone, an unexpected byproduct formed which we determined to be a 1,2-bisphenylhydrazone. We employed NMR spectroscopy to propose a mechanism of 1,2-bisphenylhydrazone formation from keto amides and phenylhydrazines. This study aims to optimize the synthetic procedure and determine the limitations of our method. We anticipate that this work will lead to a generalized synthesis of 1,2-bisphenylhydrazones.

Asymmetric synthesis of voglibose : an anti-diabetic compound

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Among the carbasugar family, several molecules have demonstrated interesting biological properties, notably valiolamine and its derivatives. Usually, these compounds are synthesized from the chiral pool.
Commercially available since 1994, voglibose, the most known synthetic derivative of valiolamine, is now one of the three leading anti-diabetic compounds in the alpha-glucosidase inhibitor family.
A concise asymmetric synthesis of voglibose was produced from an O-arylated lactic acid derivative in only 7 steps. This approach was based on an oxidative phenol dearomatization process promoted by a hypervalent iodine reagent in agreement with the aromatic umpolung concept leading to the rapid formation of an advanced key intermediate. Every stereocenter was produced during the synthesis from an inexpensive chiral auxiliary. This project, reliable to the atom economy concept, fits perfectly with the current development of green chemistry, which is attracting considerable attention in many research areas (processes, synthesis methodology).

[2+2] Photocycloadditions to Form Cyclobutanes and Bicyclo[2.1.1]hexanes Employing Copper-Based Photocatalysis

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A first-row transition metal complex, Cu(dmp)(DPEPhos)BF_4, promotes the synthesis of boracyclobutanes (11examples, 38 → 87%) and 2-oxa-BCHs (10 examples, 55 → 90%) via photocatalytic [2+2] cycloaddition. Computational analysis predicted the structures of the major and minor isomers of both processes. The catalyst structure was determined through screening of a variety of diimine and bisphosphine combinations that enabled optimization of a range of triplet energy levels, excited-state lifetimes, and photostabilities. The use of the Cu(dmp)(DPEPhos)BF_4 complex offers a mild alternative to reaction conditions employing UV light or iridium-based photocatalysts previously reported andvalidates the potential for copper-based photocatalysis for the preparation of skeletons for drug development.

Using Small Dipeptide Molecules to Explore Driving Forces of Liquid-Liquid Phase Separation.

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From the internal diffusion of cellular components to the formation of organelles, the most relevant phase separation process in biological systems involves the dehydration of molecules while simultaneously maintaining a sufficient degree of coordinated waters to possess liquid-like properties. Known as liquid- liquid phase separation (LLPS), research has been primarily directed toward large molecular weight compounds, with hypotheses often borrowing from polymer science and distinctions between compounds that can and cannot phase separate, focusing on correlational features. Due to LLPS being a process focused on hydration and morphology, accurate description, either experimentally or computationally, can be challenging to resolve for proteins and polymers. By focusing on small LLPS peptides, we can increase the experimental resolution from the monomer down to the effect that individual functional groups play in maintaining this delicate balance of partial hydration. Looking further at molecular mechanics modeling, we introduce how to model LLPS from its solvated state in solution towards a condensed state. We also explore what experimental properties can be effectively predicted and where current modeling fails to reproduce experimental results.

Co-cultivation of *Aspergillus terreus* and *Myxococcus xanthus* induces the production of antimicrobial compounds in *Aspergillus terreus.*

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Co-cultivation is a promising strategy for activating silent biosynthetic gene clusters (BGCs) in microorganisms, which usually remain inactive under standard laboratory conditions. The activation can occur due to chemical defence mechanisms or microbial communication. Our objective was to isolate and characterize antimicrobial natural products produced by *Aspergillus terreus* (saprotrophic fungi) through co- cultivation with *Myxococcus xanthus* (a predatory Gram-negative bacteria). In this study, dead *M. xanthus* cells were added to a 1-liter culture of *A. terreus,* with kanamycin included to suppress bacterial growth. The chemical profiles of the co-culture of *A. terreus* and *M. xanthus,* and the monoculture of *A. terreus* were compared using high-performance liquid chromatography (HPLC). The antimicrobial activity of the isolated compounds was assessed using spot-on-lawn assay, and their structures were elucidated via spectroscopic methods. The co-cultivation of *Aspergillus terreus* and *Myxococcus xanthus* led to the upregulation of antimicrobial compounds, which were not produced at the same levels in the monoculture of *A. terreus*. This indicates that *A. terreus* likely produced these compounds as a defensive response when co-existing with *M. xanthus* in the same environment.

EVclo: An expansion of the modular cloning synthetic biology Yeast Tool Kit for engineering designer extracellular vesicles

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Concordia University

Extracellular Vesicles (EVs) are natural Lipid NanoParticles produced by every cell known. Enabling intercellular communication over distance, EVs exist in all bodily fluids, and cell and microbiological culture media. EVs carry every biological macromolecule class, decorating the outer lipid bilayer, spanning the EV membrane, or protected in the EV lumen. Engineering designer EVs involves altering them after isolation or genetically engineering producer cells. We use synthetic biology to engineer S.cerevisiae yeast cells to produce designer EVs, building on the Yeast Tool Kit, a well-characterized biological part library and assembly standard. We designed, built, and tested a panel of EVtags,
proteins intended to force cargo to EVs. Our EVtag set included human and yeast EV proteins. Using GFP as test cargo, plate reader wells with ~10^8 EV particles reliably show GFP signals corresponding to low nanomole fluorescein standard. Nanoflow cytometry indicates few, but detectable, GFP+ particles, refining bulk measurements, and Nanoparticle Tracking Analysis and Electron Microscopy
indicate size and concentration of isolated EV particles is unchanged across engineered and wildtype strains. Our yeast EV engineering first iteration was successful; we can genetically drive EV cargos to detectable levels. We look forward to helping realize the potential of designer EVs!

Expression profiles of modified histones suggest efficient epigenetic control in hibernating ground squirrels

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Thirteen-lined ground squirrels (*Ictidomys tridecemlineatus*) are obligate hibernators capable of reducing their metabolic rates by up to 99% during winter. Their ability to remain dormant without food for an extended period in cold conditions has made them compelling subjects for research. Since some hibernators can swiftly undergo such profound changes without external cues, it has long been suggested that the ability to hibernate is driven by genetic mechanisms. Thus, we investigated the differential expression of 24 modified histones (MH) in the livers of torpid and euthermic free-ranging ground squirrels by immunoblotting nuclear extracts ($p < 0.05$). We identified the torpor-responsive downregulation of multiple permissive MHs (H2BK5ac, H3K18ac, H3K23ac, H3K27ac, H3K4me2, H3K4me3, H4K20me1, H4R3me2s), including total H3 and H4, while the linker histone H1.0 was the only histone species that was upregulated. Further, the expression patterns of total and MHs suggest previously undiscussed epigenetic strategies of torpor. Our findings corroborate the working hypothesis in the field and elucidate the integral role of epigenetic mechanisms in hibernating ground squirrels.

Reversing resistance using sequential antibiotic therapy

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Application of two antibiotics one after the other in a sequence has shown promise in slowing down resistance evolution and reducing treatment side-effects while remaining comparable in efficacy to combination therapy. In this study, we ask if sequential therapy can be used to reverse resistance: if resistance evolves to drug A, can drug B be used next to resensitize bacteria to A? Using high-throughput laboratory evolutions and screening, we show that certain A-B antibiotic pairs can reduce resistance to drug A when drug B is applied, but complete resensitization below resistance breakpoints remains rare. We extend our evolutions and screening to A-B-C tripartite drug sequences to show that complete resensitization to drug A can be reliably achieved when certain drugs are applied in an appropriate order. Genomic analyses of strains from different stages of evolutions allows us to track evolutionary trajectories that lead to resensitization over multidrug resistance and shed light on the mechanisms of resensitization. We propose that informed sequential therapy may enable reuse of antibiotics that failed due to resistance.

Developing an anillin inhibitor for the treatment of liver cancer

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Cytokinesis occurs at the end of cell division due to the ingression of a contractile ring, which cleaves the cell into two daughters. Anillin positions the ring and is recruited by active RhoA. Anillin is overexpressed in liver cancers, and an inhibitor could be developed as a targeted therapy. Depleting anillin in mice caused liver tumour regression and restoration of healthy tissue function. However, siRNAs are difficult to deliver, therefore a compound that inhibits anillin function would be desirable. Thus, compounds were designed that could disrupt the anillin-RhoA binding interface. ~40 compounds were screened using bimolecular complementation of Venus, a yellow fluorescent protein *in vitro*. Fluorescence is reconstituted when two halves of Venus interact. To find compounds that disrupt anillin-RhoA binding, we generated recombinant proteins containing anillin's RhoA-binding domain and active RhoA fused to the C-terminal and N-terminal halves, respectively. 10 uM of C1089 reduced fluorescence by ~60% and caused changes in anillin concentration in cells. Notably, 10-100 uM of C1089 increased lethality of HepG2 (hepatocellular carcinoma) cells, but not in HeLa cells (cervical adenocarcinoma), showing that it is selective for liver cancer. New derivatives are being generated and screened to find one with the potential for *in vivo* use.

Characterizing Probiotic Yeast Extracellular Vesicles

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Extracellular vesicles (EVs) are becoming recognized for their potential immunomodulatory role in shaping host-pathogen interactions. Probiotic yeasts are known to inhabit the gut as normal constituents of the human microbiome and are currently prescribed to some patients to reduce symptoms associated with gut inflammation. However, potential involvement of EVs in anti-inflammatory responses elicited by probiotic yeasts has not been explored. Here we investigate the biology of fungal EVs produced by three industrially relevant, probiotic yeast species: *Saccharomyces cerevisiae, Saccharomyces boulardii,* and *Kluyveromyces marxianus*. Initial characterization reveals differences in EV particle titers, size profiles and protein contents. EVs released during thermotolerance conditioning from one yeast species provided protection against heat stress to another, suggesting they are capable of mediating interspecies communication. Similarly, we show that EVs released from all yeast species are be taken up by cultured human cells (HEK-293) without affecting viability. Finally, we treated human THP-1 monocytes with probiotic yeast EVs and measured cytokine release to assess their potential immunomodulatory capacities. Overall, we conclude that probiotic yeast release EVs capable of interspecies communication and immunomodulation. Because these species are commonly used in biomanufacturing, these features suggest that they may be valuable for therapeutic EV production.

Stress-Induced Natural Product Biosynthesis

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Antibiotic resistance has become increasingly commonplace in many pathogenic bacterial strains. A new method of finding antibiotics is needed to match the increasing demand. To increase natural product production and identify cryptic antibiotics we have induced intracellular stress, conjugating activator plasmids into a wide range of environmental bacterial strains. This led to a significant increase in the number of isolates producing antimicrobials. I will now identify the plasmid elements, such as gene insert length and genetic makeup, that have the greatest impact on plasmid induced stress and natural product production via qPCR and LCMS. The untapped biosynthetic potential of bacteria is vast, and through this work I will explore their metabolome and uncover new potentially life saving compounds.

Optimizing Acid Tolerance in *Kluyveromyces marxianus* for Bioproduction through CRISPR-AID Screening

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Organic acids are widely used in manufacturing due to their potential for polymerization into industrial compounds. Currently, many of these organic acids are derived fossil fuels in energy intensive and polluting processes. To mitigate these environmental concerns, our group is engineering the yeast *Kluyveromyces marxianus* to act as a platform for organic acid biosynthesis from renewable feedstocks. With its broad substrate range, thermotolerance to 50°C, and acid tolerance to pH 2.5, *K. marxianus* is an ideal host. Our goal is to convert lactose from milk permeate, a waste product, into fumarate, a valuable dicarboxylic acid.

To support this, we developed a CRISPR-AID toolkit for gene activation, interference, and deletion, enabling both rational design and high-throughput screening. We have designed a CRISPR-AID genome-wide guide library to provide a versatile resource for phenotype screening. When screened on high concentrations of fumaric acid, we identified several hits, including activation of multidrug transporters, cell wall remodeling, and previously uncharacterized genes. We are currently validating these hits in a Cas-free system and investigating their role across organic acids.

Through these efforts, we aim to establish *K. marxianus* as a sustainable platform for organic acid production.

Comparing aptamer properties for binding T cells

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T cells are an important component of the adaptive immune system and a useful target for therapeutic and diagnostic applications. Thus, developing ligands against them is of great interest with robust single-stranded nucleic acids (i.e., aptamers) offering unique advantages. Indeed, aptamers offer affinities and specificities on par with antibodies, while also having lower production costs and greater stability. However, there is a lack of studies offering head-to-head comparisons of these aptamers. To this aim we compared several aptamers reported to bind to unique T cell receptors (CD3, CD4, and CD8). Using secondary cell lines, the apparent affinity and specificity of each aptamer were characterized through flow cytometric analysis. Of the aptamers evaluated the apparent affinities differed from what was reported in the literature by 10-100-fold. Only one aptamer, against CD8, showed significant non-specific binding to its target. We then looked to improve the binding of CD3 and CD4 binding aptamers through modifications to buffer composition and incubation temperatures. Results showed reduced binding affinities in each case, illustrating the importance of buffer composition for aptamer function. Our first head-to-head comparison demonstrates the need for more robust aptamer validations to make use of their advantageous properties.

Enzymatic PET depolymerization without bulk water: a novel approach to plastic recycling

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McGill University

Enzymatic polyethylene terephthalate (PET) depolymerization has emerged as a promising alternative to traditional “recycling” methods. This approach boasts improvements in ecotoxicity and a reduced reliance on fossil fuels when compared to the production of virgin plastic. However, recent life cycle analyses have illuminated that enzymatic recycling still leaves a larger environmental footprint than direct PET production from fossil fuels due to the energy-intensive amorphization of the plastic prior to the reaction, using sodium hydroxide for pH maintenance, and significant wastewater generation.

Our group has taken an innovative approach: mechanoenzymatic PET depolymerization, which operates without bulk water and using intermittent mechanical mixing. Unlike dilute conditions, this technique progresses equally on both the crystalline and amorphous plastic regions, avoiding any harsh chemical or thermal pre-treatment. The limited water use prevents terephthalic acid, the depolymerization product, from dissolving and affecting the pH, eliminating the need for sodium hydroxide addition, while also significantly reducing the amount of wastewater. Recent breakthroughs demonstrate our capability to achieve complete depolymerization of highly crystalline PET, highlighting the potential of our technology as a more environmentally friendly alternative to current processes.

This presentation will delve into our recent investigations into the mechanism behind reactions in this water depleted environment.

Using Oriented Peptide Array Libraries (OPAL) to Identify Novel Binding Peptides for Dual Lysine and N-terminal Methyltransferase METTL13

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Methyltransferase-like protein 13 (METTL13) is a dual methyltransferase which catalyzes the dimethylation of lysine 55 (K55) and the trimethylation of N-terminal glycine (G2) on eukaryotic elongation factor 1A (eEF1A). eEF1A is an elongation factor involved in translation, and its modulation can result in direct effects on overall protien synthesis within a cell, a common characteristic of tumour microenvironments. An upregulation of METTL13, as well as an increase in methylated forms of eEF1A, has been observed in a number of cancer types. Its implication in disease highlights the canonical function of METTL13 as a potential avenue for therapeutic development.

To tackle this, oriented peptide array libraries (OPAL) were used sequentially to generate novel METTL13 binding peptides from degenerate sequences. As a result, 43 binding peptides were identified. These binding peptides were assayed with METTL13 *in vitro* to determine which peptide binding disrupts METTL13 enzymatic activity. Of the 43 tested, 6 peptides displaying inhibition were selected for dose-response curves and IC50, and the most significant inhibitors were then used to create permutation arrays. These were them used to inform both sequential and physiochemical binding motifs for potential METTL13 inhibitors, which will be used in further peptide therapeutic development for METTL13.

Development of a capture-based method for separation of riboswitch conformational states

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McGill University

Riboswitches are structured non-coding RNA elements that regulate bacterial gene expression by switching conformation in the presence of specific small molecule ligands, making riboswitch disruption an attractive approach for antibacterial drug development. Currently, very little is known about how riboswitch sequence mutations impact binding of native ligands or inhibitors and downstream changes in conformational switching. To explore the mutational landscape of riboswitch binding and conformational change, we developed a capture-based method to partition distinct conformational states. Here, I will present the capture and release of a *yitJ* SAM-I riboswitch mimic from DNA probes conjugated to magnetic beads. To improve the capture and release assay, we also developed a Surface Plasmon Resonance (SPR) method to screen DNA probes that are more efficiently "displaced" during riboswitch switching. The DNA probes with the best displacement will subsequently be attached to magnetic beads, allowing for separation of riboswitch conformational states. Our work will ultimately be used to screen mutated riboswitch libraries in the presence of native and novel ligands to uncover crucial nucleotides for structure switching.

De novo resistance to "evolution-proof" Oct-TriA1 in *E. coli BW25113*

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Concordia University

Studies on new antibiotics often include evolution experiments to assess resistance rates or mechanisms of action. Some antibiotics show little to no resistance evolution and are termed "evolution proof", making them promising candidates for next-generation therapies. However, the evolutionary resilience of these compounds is largely known through a limited array of Adaptive Laboratory Evolution (ALE) experiments, and has generally not been independently verified. OctTriA1 is one such antibiotic, against which laboratory evolution experiments have failed to describe *de novo* resistance. The tridecaptins are a group of non-ribosomal lipopeptides that are active against Gram-negative bacteria binding to lipid II and disrupting the proton motive force. We describe here the first reported evolution of *de novo* resistance to Oct-TriA1. This presentation will discuss these findings, emphasizing the implications for our understanding of resistance mechanisms and the potential design of new
antimicrobial strategies that could target these newly identified pathways. It will also revisit the concept of "evolution proof" antibiotics, challenging the notion and underscoring the importance of rigorous, innovative experimental approaches to predict and combat resistance effectively.

Unravelling the role of lipid peroxidation in bacterial membrane vesicle formation via fluorescence microscopy

F. Fungo
McGill University

Bactericidal antibiotics have been recently shown to include cell death via the production of reactive oxygen species (ROS). However, bacteria have developed multiple mechanisms by which they can survive exposure to antibiotics, where the formation of membrane vesicles (MVs) plays a key protective role. To investigate the link between antibiotic-induced ROS and MV formation, we developed a fluorescence imaging platform that capitalizes on a highly sensitive fluorogenic ROS sensor. Our methodology allowed us to correlate levels of ROS production with ensuing morphological changes and damage undergone by *E. coli*. Notable morphological changes observed include bacterial membrane blebbing and expulsion of MVs. By modulating the level of ROS production and equipped with our fluorogenic ROS sensor, we show that lipid peroxidation triggers the formation of MVs, the latter acting as a reservoir of oxidizable lipids. Importantly, we report key observations relating to the morphological response of *E. coli* to oxidative stress as a function of ROS levels.

Developing Enzyme Cascades and Cell-free Strategies for Protein Engineering

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Protein engineering focuses on designing novel or improved enzymes for diverse applications, including biocatalysis, therapeutics, diagnostics, and pharmaceuticals. This field has evolved with techniques such as directed evolution and rational design, which rely on screening mutant libraries to enhance enzyme activity, specificity, and efficiency. Coupled enzyme assays and multi-enzyme pathways have emerged as effective strategies for measuring enzyme activity, facilitating rapid and efficient screening. Recent advancements in engineering oxidoreductases have shown their significance as biocatalysts, facilitating electron transfer in enzymatic reactions. These enzymes often utilize nicotinamide adenine dinucleotide (NAD) or nicotinamide adenine dinucleotide phosphate (NADP) as cofactors, which can function as either electron donors (NADH or NAD(P)H) or acceptors (NAD or NADP+). While traditional methods for measuring NAD(P)H concentration, such as absorbance at 340 nm, can assess enzyme activity, their sensitivity may be insufficient for low-concentration assays. This study focuses on developing a fluorescence-based coupled enzyme cascade reaction to enhance the screening of redox enzymes. By leveraging the NADH/NAD+ redox reaction, our approach integrates fluorescence readouts, offering greater sensitivity and enabling high- throughput, efficient, and continuous assays for biocatalytic enzyme activity. This innovative methodology
aims to improve the detection of NAD(P)H/NAD(P)+-dependent oxidoreductases, advancing the field of protein engineering.

Designing the first liquid-liquid phase separating short peptides that evade irreversible amyloid-like fiber formation

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McGill University

Short peptides are an exciting new single-component (simple) coacervate material. Unlike complex coacervates that form through electrostatic effects, short peptide coacervates undergo liquid-liquid phase separation (LLPS) due to hydrophobic effects, hydrogen bonding, and π-π stacking. These coacervates are significantly more hydrophobic than complex coacervates, opening the door to transition metal catalysis in aqueous environments. Initial studies proposed a diphenylalanine motif (FF) as a driving force for LLPS. Unfortunately, this motif is also known to induce irreversible amyloid fiber formation. This study explores the necessity of π-π stacking — particularly in the FF motif — for LLPS of short peptides. We demonstrated that by modifying the FF motif, not only do we still observe LLPS, but in some instances, fiber formation can be averted.

Synthesis of Fluorogenic Substrates for Gliomas

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Gliomas are a classification of primary brain tumours, accounting for 30% of all cases with 80% of those being malignant. The standard of care often begins with surgical resection whereby the surgeon uses pre- operative scans as a guide to identify the cancerous tissue that should be removed. However, surgery has shortcomings related with the reliability of detecting low grade tumours due to their small size and diffuse margins. Thus, a solution to overcome these issues is to use fluorescence-guided surgery which utilizes cancer-selective fluorophores to enhance the real-time detection of tumours intraoperatively, overall reducing cancer recurrence post-surgery, and thereby improving a patient's prognosis.
Herein, I will report an enzymatic approach to the synthesis of fluorogenic substrates for relevant glioma enzymes. Notably, the application of L-amino oxidase derived from snake venom opens doors to access distally modified α-ketoglutaramate analogues. Synthesis, characterization, and preliminary assays will be shown as well as future directions of this project.
Overall, the significance of this research is the development of a fluorescent chemosensor for gliomas, serving as a novel diagnostic tool with applicability in fluorescence guided surgery. The project aims to fill a gap in the currently available treatment for glioma patients.

Mechanism of action of the MacAB-TolC multidrug efflux pumps in antimicrobial resistance

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Bacterial multidrug efflux pumps (MEPs) are membrane protein complexes that contribute to antimicrobial resistance by transporting antibiotics out of bacteria. This occurs through the utilization of cytosolic energy sources to drive conformational changes that are coupled to drug efflux. Of the many MEPs, my interest lies with the MacAB-TolC efflux pump as it plays a role in tigecycline resistance in the critical priority pathogen
A. baumannii. This project will focus on how ATP binding/hydrolysis is coupled to cytoplasmic conformational changes and drug efflux in MacAB-TolC.
Promising labeling positions of MacB that demonstrate distance changes between open and closed conformations have been identified, in order to be mutated to a cysteine without disrupting protein function. MacB will then be labeled using cysteine-specific chemistry to monitor conformational changes upon the addition of different nucleotides and antibiotics using fluorescence changes and FRET.
This project is expected to reveal nucleotide-dependent conformational changes that drive drug efflux in the cytoplasmic domains of MacB. This work will provide insight into the potential characterization of mechanisms in other tripartite efflux pumps and to assist in designing small molecule inhibitors that could disrupt its mechanism of action.

Modulation of amyloid aggregation and associated toxicity with polyphenolic gallotannins

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Amyloidogenic diseases involve protein misfolding and aggregation into insoluble amyloid deposits, impairing organ function. These deposits are linked to diseases like Alzheimer's, Parkinson's, and type 2 diabetes (T2DM). T2DM is characterized by the pancreatic deposition of islet amyloid polypeptide (IAPP), a peptide hormone crucial for glucose regulation by controlling satiety levels and gastric emptying. However, IAPP can misfold, forming cytotoxic aggregates in pancreatic islets, leading to β-cell dysfunction. Thus, targeting IAPP aggregation is a promising strategy for treating T2DM.
Natural gallotannins are potential amyloid modulators, though their effects on amyloid self-assembly are not fully understood. This study examines two gallotannins, corilagin and β-TGG, and their inhibitory effects on IAPP aggregation. Using thioflavin T fluorescence, atomic force microscopy, and circular dichroism, it was found that the gallotannins delay IAPP self-assembly and reduce fibril length and quantity. Cytotoxicity was assessed by monitoring cell metabolism, LDH release and ROS production. Corilagin showed significant cytoprotective properties on INS-1E pancreatic cells against IAPP toxicity and membrane damage. Peptide- gallotannin interactions were further investigated using all-atom explicit solvent molecular dynamics simulations, revealing hydrogen bonds and π-π stacking interactions. These findings highlight the potent anti- aggregative properties of gallotannins, suggesting their potential as a basis for developing anti-amyloid agents.

Development of a Long-Wavelength Photocaged β-Lapachone for Enhanced Tumor Penetration and Activation

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β-Lapachone is a quinone with potent anti-cancer properties, particularly effective against cancers overexpressing NADPH Quinone Oxidoreductase 1 (NQO1), such as pancreatic, prostate, and breast cancers. Its mechanism involves a futile redox cycle catalyzed by NQO1, producing reactive oxygen species (ROS) that induce cancer cell death. However, β-lapachone's clinical potential is limited by a short half-life (~20 minutes) and adverse effects, including methemoglobinemia, which hinder its pharmacological application.
To address these issues, we developed a prodrug version of β-lapachone by attaching a coumarin-based photoremovable protecting group, or "photocage." This modification inactivates the compound, preventing methemoglobinemia and extending metabolic stability (>2 hours). Light activation releases β-lapachone, restoring its cytotoxic activity specifically in NQO1-expressing cells.
Despite promising results, the 420 nm light required for photo-uncaging suffers from limited tissue penetration (~1-2 mm), restricting in vivo application in tumors. Here, we present the synthesis and characterization of a new photocaged β-lapachone that absorbs at a longer wavelength, enhancing tissue penetration and activation at the tumor site. This approach holds potential for more effective cancer treatment in clinically relevant models.

Exploiting Cytochrome P450 Promiscuity through the Chemoenzymatic Synthesis of Bicyclic Seongsanamide B

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University of Ottawa

We are investigating the promiscuity of a cytochrome p450-catalyzed biaryl ether cyclization through the chemoenzymatic synthesis and derivatization of the bicyclic depsipeptide, seongsanamide B. This bacteria- derived antiallergenic contains a thioesterase-driven macrolactone ring, along with a cytochrome p450- catalyzed biaryl ether cyclization.[2] While most reported p450-catalyzed transformations occur during biosynthetic assembly on enzyme-linked substrates, seongsanamide B uniquely has its transformation post- assembly, on the carrier protein-free substrate.[4,5] This suggests that this p450 has potential to be a versatile biocatalyst capable of catalyzing substrates beyond seongsanamide B.
We have previously established that treating the linear intermediate with its native thioesterase produces the monocyclic precursor, seongsanamide E.[3] We now attempt the subsequent transformation of the monocycle with the native cytochrome p450 to catalyze the oxidative phenolic coupling to form the biaryl ether- containing bicyclic seongsanamide B. We are also interested in an enzymatic cascade, transforming the linear intermediate to the final bicyclic product with a one-pot incubation of its native thioesterase and cytochrome p450. The promiscuity of this enzymatic transformation will be probed using synthetic analogs of its precursors.

Deciphering the regulatory role of TANGO2 in CoA metabolism

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TANGO2 deficiency disorder (TDD) is a neurometabolic condition characterized by recurrent metabolic crises, cardiac arrhythmias and rhabdomyolysis. While the function of TANGO2 remains elusive, emerging evidence suggests its involvement in lipid metabolism and mitochondrial function. Previous studies revealed that TANGO2-deficient cells accumulate triglycerides and exhibit altered lipid droplet morphology, hinting at a lipid imbalance as a contributing factor to TDD. Interestingly, patients taking vitamin B5, a precursor to coenzyme A (CoA), have shown improved management of neurological symptoms and metabolic crises. This raises the hypothesis that TANGO2 plays a role in CoA metabolism, possibly by interacting with intermediates in the CoA salvage pathway. We demonstrated cells lacking TANGO2 have reduced levels of CoA and its precursor, phosphopantetheine, during starvation, supporting a connection between TANGO2 and CoA biosynthesis. Using protein-metabolite interaction assays and enzyme activity studies, this project aims to elucidate the mechanistic role of TANGO2 and its relationship to lipid homeostasis. Moreover, the hypothesis that TANGO2 is involved in mitochondrial import and function will be tested through mitochondrial purification assays and proteinase K treatments. This research could shed light on the pathophysiology of TDD and uncover potential therapeutic approaches, including the use of vitamin B5, to alleviate disease symptoms.

Unveiling the Kinetic Tango: Exploring G-quadruplex Ligand Binding Dynamics and Transfer Mechanisms for Enhanced Therapeutic Strategies

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Guanine quadruplexes (G4s) are non-canonical nucleic acid secondary structures, thought to play critical in- cell regulatory roles. Notably, G4-containing genes have been implicated in oncogenesis, making them potential targets for therapeutics. Small molecules, such as porphyrins, can interact with G4s, modulating their stability and function. In this context, the binding kinetics are particularly important as they determine the bound lifetime of G4-ligand complexes. This in turn governs how the ligand finds its in- cell target and the extent to which it becomes trapped in off-target complexes.
In this study, we utilize NMR and SPR techniques to measure the binding kinetics of G4s with the porphyrin TMPyP4. We found that the kinetics were extremely slow, to the extent that the ligand is effectively trapped onto the first G4 structure encountered. However, these rates increased dramatically as the G4 concentration increased. Further analyses elucidated a mechanism in which ligands are transferred directly between G4s via collisions in solution. Such a pathway mimics facilitated diffusion in protein-DNA interactions through which ligands can rapidly reach intended quadruplex targets by utilizing more readily available neighbouring dsDNA. This has potential implications for the development of G4-binding ligands which can capitalize on this direct transfer for enhanced therapeutic activity.

Engineering the biosynthesis of natural glycosylated natural products

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Glycosylated natural products (GNPs) have a range of applications in multiple industries, making their manufacturing a valuable endeavour towards compound discovery. These molecules are formed through the glycosylation of an activated sugar donor and a non-sugar moiety, or aglycone, by enzymes named glycosyltransferases (GTs). Using GTs, new-to-nature GNPs can be generated by mixing and matching aglycones and sugar donors. Producing these new GNPs is however set back by two obstacles: the availability of sugar donors is limited by the fact their enzymatic pathways are difficult to recreate and modify in a laboratory setting, and wild-type GTs have limited efficiency in performing novel GNP synthesis. In this work, an *in vitro* enzymatic pathway towards the production of dTDP-acosamine, an new-to-nature sugar donor, has been developed. Furthermore, GT engineering tools are being developed. Through *in silico* modelling, characterization of a GT known as AknS and its helper protein (AknT) has been performed—the pair being attractive for engineered biosynthesis of epirubicin. These endeavours should allow the creation of *in vitro* tools for glycorandomization, by swapping enzymes in the established pathway to create new sugar donors, as well as develop new GTs able to perform these new-to-nature reactions.

Enhancing Aptamer Diversity for Targeted Therapeutics Using DNA-Encoded Libraries

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Polymers with sequence definition offer a transformative approach to aptamer development by allowing access to programmable morphologies and applications. Traditional aptamers face limitations like modest binding capabilities and rapid degradation. Our research utilizes high-throughput identification of effective protein target-recognition molecules using DNA-encoded libraries of chemically diverse sequence-defined oligomers, termed "alenomers" (Aptamer-Like ENcoded OligoMERs), generated on an automated DNA synthesizer. By integrating nucleosidic and non-nucleosidic components into our alenomers, we unlock new interactions for biomolecule binding and enhance binding efficacy.

We synthesized a library of approximately 300,000 DNA-encoded alenomers using a split-and-pool method for efficient target selection. Our approach successfully identified modified aptamers with improved binding and stability against thrombin. The study further aims to develop novel aptamers targeting key proteins, which plays a critical role in cancer progression. This research has the potential to redefine nucleic acid- based therapeutics, expanding the utility of aptamers in clinical settings and offering significant implications for precision medicine and complex disease treatment.

By addressing the need for selective and robust aptamers, our work aims to enhance targeted therapies' efficacy and provide a robust platform for next-generation biomedical solutions.

Unveiling the interaction of cationic antimicrobial peptides with gram-positive bacterial cell walls

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A report on the economic impact of antibiotic resistance predicts that by 2050, antimicrobial resistance could cause up to 10 million deaths annually. Rising resistance due to overuse of current antibiotics and a lack of new drug discoveries have prompted research into alternative therapeutic strategies using cationic antimicrobial peptides (cAMPs). Due to their non-specific mechanism of action, cAMPs remain effective despite bacterial adaptation. While their lytic action on bacterial lipid membranes is well known, their interaction with the protective cell wall remains less explored. This study investigates how cAMPs interact with the complex cell wall of the model Gram(+) bacterium *Bacillus subtilis*, which contains peptidoglycan (PGN) and negatively charged phosphate rich wall teichoic acids (WTAs). Using solid-state nuclear magnetic resonance (ss-NMR), we examined three cAMPs—Aurein 1.2, Caerin 1.1, and DMS-DA6-NH2. We compared ^{31}P spectral line shapes and relaxation times of the cell wall in the presence and absence of cAMPs, revealing interactions with the phosphate groups of the WTAs. Additionally, ^{13}C ss-NMR revealed alterations in carbohydrate dynamics. Similar changes were noted in *Staphylococcus aureus*, a key pathogen, with DA6. These findings indicate that cAMPs interact with Gram(+) bacterial cell walls, particularly WTAs, expanding our understanding of their antimicrobial action.

Synthesis of Oligonucleotide Conjugates Containing Selenium Modified Linkers

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Oligonucleotide conjugates hold therapeutic potential by enhancing targeted delivery, cellular uptake, and stability. These conjugates range from simple molecules like cholesterol to complex peptides. However, their synthesis faces challenges due to incompatibilities between ligation partners. Our lab recently developed a reductive diselenide-selenoester ligation (rDSL) method to efficiently prepare DNA-peptide conjugates. This process uses a 5'-diselenide cross-linked DNA dimer and a C-terminal selenoester peptide for efficient ligation.

In this study, we synthesized alkylene linkers with a terminal 2-cyanoethyl protected selenium for solid-phase coupling to the 5'-end of an oligonucleotide. After deprotection and cleavage from the solid support, 5'- diselenide cross-linked DNA dimers were evaluated. Linkers with 4- and 10- carbon atom alkylene chains between the selenium and DNA were prepared. Efficient dimer formation was observed for the longer chain, confirmed by denaturing polyacrylamide gel electrophoresis. Future work will focus on functionalizing 5'- diselenide cross-linked DNA with other molecules and extending this method to RNA and modified oligonucleotides. Developing more efficient synthesis strategies will advance the therapeutic application of oligonucleotide conjugates.

Self-assembly of Nanostructures via the Hydrophobic Effect and DNA Base Pairing

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DNA nanotechnology is a novel method of organizing matter using precise AT and CG base-pairing. This self-assembly language is relatively simple and makes the final morphology fully predictable. Precise control over the size, shape, and surface patterning in DNA nanostructures plays an important role in their biological activity, making it a promising drug delivery system for nucleic acid therapeutics, such as siRNA and antisense oligonucleotides. However, complex DNA-based nanostructures face stability challenges because of their high DNA density and large number of unique strands, making it time-consuming to ensure the safety of all the sequences before market release.

Inspired by protein self-assembly, which employs different interactions, our approach incorporates hydrophobic polymers into DNA nanostructures. This allows them to self-assemble in a hierarchical and stepwise manner, much like proteins. This makes the nanostructures more programmable, enabling the generation of multiple structures with different morphologies with similar building blocks. This expands the design space of DNA nanotechnology. This method also reduces the need for numerous different DNA sequences and lowers the overall DNA density, ultimately enhancing the drug delivery applications of DNA nanostructures.

Mechano-enzymatic depolymerization of highly crystalline polyethylene naphthalate under moist-solid conditions

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To reduce the pollution of plastics and expand their prospects, scientists are putting their efforts into the development of new biodegradable plastics and of closed-loop plastic recycling technologies. Enzymes are especially attractive catalysts for plastic depolymerization because they are selective, non-toxic, renewable and biodegradable. The Auclair lab has recently demonstrated that many enzymes can be more active in moist-solid mixtures than in traditional aqueous conditions. This was first explored as a means to better mimic the natural environment of secreted enzymes but was also found to be advantageous with poorly soluble substrates such as biomass and plastics, while minimizing wastewater. This unique methodology is optimal when the moist-solid reaction mixture is intermittently mixed by mechanical means, hence it is also referred to as mechano-enzymology. Remarkably, when applied to the enzymatic depolymerization of PET, this technique not only proceeds with higher yields than in bulk water, but also enables the direct depolymerization of high crystallinity PET, which normally requires an initial amorphisation step. This presentation will focus on the mechano-enzymatic depolymerization of an even more recalcitrant synthetic polymer, polyethylene naphthalate (PEN), with insights from mechanistic and kinetic studies.

One Assay to Read-through all: a new high-resolution, high-throughput nucleic acid polymerase read-through assay.

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G-quadruplexes (G4s) are non-canonical DNA structures which have been implicated in cancer biology and are attractive drug targets. G4s are typically composed of four G-tracts of three or more consecutive deoxyguanosine residues that come together to form stacked planar G-tetrads. The biological activity of G4s is related to their ability to block the progression of DNA polymerase enzymes, influencing replication and gene transcription. Current assays to detect polymerase blockage involve gel electrophoresis making them low resolution and low throughput. Thus, we currently lack the detailed kinetic information required to understand how G4 sequence, structure, dynamics, and ligand/drug binding affect their ability to block polymerases.

We developed a new high-resolution, high-throughput polymerase blockage assay that can provide critical information on the interaction of non-canonical nucleic acid structures with DNA polymerases. The assay utilizes a fluorescence probe and quencher to track the progress of polymerase read through using a plate- reading fluorimeter. The assay is currently being used to explore the effects of G-quadruplex structure, namely loop length and bulges, on polymerase read-through. The developed assay will allow us to form a comprehensive, quantitative understanding of how non-canonical DNA blocks nucleic acid polymerases and how these interactions can be modulated by potential drugs.

Effects of flanking regions on DNA i-motif folding and stability

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i-Motifs (iMs) are four-stranded non-canonical nucleic acid secondary structures that are formed by cytosine- rich sequences. Putative i-motif forming sequences are concentrated in human promoter and telomeric regions, suggesting possible biological roles. However, many iMs do not readily fold at neutral pH, stimulating many studies in the stabilization of iMs. To date, the influence of flanking nucleotides on iM structures has not received much attention. Here, we present a systematic study on how i-motif stabilities and folding change with flanking nucleotides. We found the mere presence of non-interacting flanking nucleotides can dramatically destabilize iM structure and slow down folding. The complementary flanking nucleotides can recapture this stability loss and, in some cases, lead to faster folding and more stable structures. A bioinformatic study on the human promoter region suggested that the flanking regions are more likely than average to be complementary to each other, suggesting that this stabilization might be biologically relevant. We analyzed several naturally occurring iM sequences and found that the complementarity of the flanking region substantially stabilized the structures (53-fold faster folding and 16 °C more stable). Our results show that the regions of DNA flanking iMs are an important and overlooked factor in iM folding and stability.

ENVIRONMENTAL CHEMISTRY

Effet du vieillissement sur les propriétés de surfaces des microplastiques : comparaison de différentes méthodes utilisées pour simuler les microplastiques environnementaux

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Dans l'environnement, les plastiques subissent une fragmentation en microplastiques (MPS) sous l'action des rayons ultraviolets (UV), par abrasion mécanique, ou via des réactions chimiques. L'altération subite au cours de leur formation introduira des groupements fonctionnels à la surface et affectera leurs interactions avec les contaminants. Pour simuler le vieillissement des MPs en laboratoire, les chercheurs ont altéré des MPs de façon accélérée par diverses méthodes. Cependant, ces MPs ne représentent peut-être pas de façon réaliste la morphologie, la distribution de la taille, et la chimie de surface des MPs environnementaux. Cette étude vise à identifier la meilleure approche pour produire rapidement des MP représentatifs des MP vieillis dans l'environnement. Les MP ont été vieillis à l'aide des UV, de l'ozone et du persulfate de potassium. Le degré d'altération fut quantifié par l'indice carbonyle et l'effet du vieillissement sur la morphologie et la chimie de surface des MP caractérisés par différentes méthodes spectroscopiques. L'adsorption de différents contaminants fut caractérisée afin de comprendre comment les différentes propriétés de surface des MP vieillissent influencent l'adsorption des contaminants. Les résultats de cette étude permettent d'identifier comment les processus de vieillissement influencent les propriétés et les interactions des MPs utilisés comme modèle des MPs environnementaux.

Effet de la présence de métaux sur l'ozonation catalytique de l'antibiotique Norfloxacine et son impact écotoxicologique

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L'effet de l'antibiotique Norfloxacine (NOF) dans des suspensions d'argile aqueuse sur l'écotoxicité du mélange réactionnel ozoné a été étudié, en tenant compte du rôle du cation échangeable pour simuler l'impact des antibiotiques libérés dans la nature et leur dégradation partielle sur la biodiversité. L'accent a été mis sur les catalyseurs à base de montmorillonites échangeuses d'ions et sur *Lemna minor*, une macrophyte aquatique sensible aux changements dans l'environnement. L'écotoxicité, évaluée selon différents critères, s'est avérée évoluer en fonction des cations échangé. La comparaison de l'activité catalytique de Fe(II)Mt avec d'autres montmorillonites a montré que le taux de dégradation et l'écotoxicité résultante dépendent fortement du type du métal incorporé. Les méthodes analytiques comme spectrophotométrie UV-Vis et LC-MS ont confirmé la génération des intermédiaires hydroxyles et la dégradation de la structure de NOF. Ces résultats sont essentiels pour comprendre le devenir des antibiotiques dans des conditions aérobies dans des matrices naturelles contenant de l'argile.

Mécanismes de séquestration et effets toxiques des ions métalliques du platine et du palladium chez l'algue verte unicellulaire chlamydomonas reinhardtii

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Dans ce travail, l'algue verte *C. reinhardtii* a été utilisée comme un organisme modèle pour investiguer l'accumulation, la séquestration et les effets toxiques des ions métalliques du Pt et du dans les cellules algales. Les cellules sont exposées pendant 72 h aux différentes concentrations nominales de Pt (0, 5, 20, 50 et 80 µg/L) et de (0, 0,5, 5, 20 et 40 µg/L). Les résultats montrent que l'effet toxique de la bioaccumulation des ions métalliques influence le taux de croissance de l'algue verte, la structure et la morphologie cellulaire ainsi que les réactions biochimiques. L'effet commence, pour l'ion, aux environs de 5 µg/L et s'accroît jusqu'à l'absence quasi-complète de croissance à partir de 40 µg/L. La $CE_{50\text{-}72h}$ obtenue est de 6.3 ± 0.3 µg/L. Pour l'ion Pt, l'effet de toxicité est peu marqué sur la croissance de l'algue. La toxicité des ions métalliques est plus importante à pH 7, elle diminue de façon significative à pH 8 et est encore plus faible à pH 4. Ce phénomène est particulièrement frappant aux plus grandes concentrations exposées. Nous avons constaté également que le provoque une toxicité plus importante que le *Pt sur C. reinhardtii.*

COMPUTATIONAL CHEMISTRY

In Silico Molecular Targets, Docking, Dynamics Simulation and Physiologically Based Pharmacokinetics Modeling of Oritavancin

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Oritavancin is a semi-synthetic lipoglycopeptide antibiotic primarily used to treat serious infections caused by Gram-positive bacteria. The aim of this work was to investigate the molecular targets, binding interactions, and pharmacokinetic profile of oritavancin. Computational methods used include target prediction, molecular docking, molecular dynamics simulation, pharmacokinetics prediction, and physiological-based pharmacokinetics (PBPK) modeling. The results of pharmacokinetics showed that oritavancin is moderately soluble in water and is not permeable across the blood-brain barrier. Target prediction analyses identified seven molecular targets in both bacteria and humans. Molecular docking results showed the highest binding affinity with PI3-kinase p110-gamma subunit (-10.34 kcal/mol), followed by Acyl-CoA desaturase (-10.07 kcal/mol) and Cytochrome P450 2C19 (-8.384 kcal/mol). Oritavancin PBPK modelling results showed that infusion has lower peak concentrations (Cmax) compared to bolus administration, with 1200 mg yielding 16.559 mg/L, 800 mg at 11.258 mg/L, and 200 mg over 3 days at 7.526 mg/L. Notably extended half-lives ($t_{1/2}$) for all doses and slightly higher clearance rates compared to bolus, particularly for the 1200 mg and 800 mg doses. In conclusion, this study corroborated existing clinical pharmacokinetic data, which confirmed the model's accuracy and predictive capability.

Computational Investigation of Water-Stable Metal-Organic Frameworks for Efficient Small-Toxic-Molecule Adsorption

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The design of advanced materials for efficient capture of toxic and harmful chemicals such as NH_3, H_2S, NO_2 and SO_2 is essential. Metal-organic frameworks (MOFs) have emerged as a promising category of sorbent materials for the capture of such toxic chemicals. However, no clear relationship has been established between the capability of the MOFs to capture toxic molecules and their properties. In this work, we investigate computationally the adsorption of selected toxic molecules on water-stable MOFs, including UiO- 66, UiO-67, MIL-53 and MFM-300. The MOF geometries and electronic properties such as bandgaps and projected density of states are determined by spin-polarized density-functional theory (DFT), along with the surface-binding motifs and energies of the small-toxic-molecule adsorbates. The Hubbard U correction is employed to properly treat *d* electrons of the transition metals and its effect on the bandgap of water-stable MOFs surveyed. DFT+U calculations not only yield results in good agreement with experimentally determined bandgaps and structural properties, but also highlight weak interactions between adsorbates and the MOFs, showing unambiguously that adsorbates bind to the MOFs investigated via hydrogen bonds to the MOF hydroxyl groups. This study provides further insight into the design of water-stable MOFs for efficient adsorption/removal of target toxic molecules.

Docking-based screening and analysis of Bisphenol A/F/S analogs with potential endocrine disrupting activity the human estrogen receptor alpha (hERα)

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We conducted a case study to assess the Nuclear Receptors (NRs) related endocrine disruption effects activity of chemicals with backbone structures similar to bisphenols, but variations in functional groups to explore the potential of molecular docking as a high throughput in silico screening tool for identifying chemicals of environmental health concern. The molecular docking analysis elucidates how modifications in functional groups, such as NH_2, Cl, and OCH_3, influence their interaction with the human estrogen receptor alpha (hERα), a key player in endocrine regulation. Through comparative docking analysis, we examined how bisphenol analogous interacted with three distinct conformations of hERα: the apo structure and structures with either an agonist or antagonist ligand bound. Our results revealed that the majority of these compounds exhibit significant to moderate binding affinity toward the human estrogen receptor alpha. While compounds like BPA exhibited partial agonist activity, stimulating hERα activity to varying degrees, other compounds displayed non-agonist behavior, suggesting a different mode of interaction with the receptor. Further analysis indicated that the presence of specific functional groups, such as hydroxyl or amine groups on the aromatic ring of these compounds, played an important role in modulating their binding affinity to hERα.

Influence of Cholesterol on the Permeation of Small Hydrophobic Gases through Lipid Membranes: Insights from Molecular Dynamics Simulations

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Cholesterol plays a vital role in modulating the fluidity and rigidity of plasma cell membranes, comprising 20-50% of animal cell membranes. It is commonly believed to reduce membrane permeability to various solutes, both hydrophilic and hydrophobic. However, the specific impact of cholesterol concentration on the permeability of small hydrophobic gases, as well as the exact mechanisms involved, remain debated topics. In this work, we employ molecular dynamics simulations to investigate the passive permeation of three highly hydrophobic and biologically relevant gases — O_2, NO, and CO — and water molecule for comparison, across mixed DPPC/cholesterol bilayers of varying concentrations. We find that while the permeability of water, a hydrophilic solute, decreases consistently with increasing cholesterol concentration, the permeability of hydrophobic gases displays a bimodal behavior. Analysis of the calculated diffusion coefficients for the latter hydrophobic gases within the membranes further reveals that they are relatively unaffected by cholesterol concentration. However, local partition coefficients at the lipid headgroups and tails are oppositely modulated by cholesterol, correlating with cholesterol-induced looser packing at the lipid headgroups and tighter packing at the lipid tails, respectively. These results provide additional insights into how cholesterol infuences the permeability of biological membranes to small hydrophobic gases.

NANOCHEMISTRY

Advancements in PMMA Nanoparticle Synthesis for Drug Delivery Applications

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The development of effective drug delivery systems remains a cornerstone of modern pharmaceutical research, with a significant focus on enhancing the precision and efficacy of therapeutic interventions. Among various strategies, the use of polymer-based nanoparticles has shown considerable promise in achieving controlled and targeted drug delivery. Polymethyl Methacrylate (PMMA) nanoparticles offer a versatile platform for drug encapsulation due to their biocompatibility and tunable properties.

This study explores the synthesis of PMMA nanoparticles utilizing the nanoprecipitation technique, a method renowned for its ability to produce nanoparticles with controlled size and distribution. Our research involves the optimization of synthesis parameters to enhance encapsulation efficiency and stability of therapeutic agents. Comprehensive characterization of the nanoparticles is conducted, including size distribution, morphology, and release kinetics, to assess their potential for targeted drug delivery applications.

The findings from this study provide valuable insights into the practical applications of PMMA nanoparticles in drug delivery, highlighting their potential to improve therapeutic outcomes through precise delivery and controlled release of active pharmaceutical ingredients.

A Novel Method for Embedding Ruthenium Nanoparticles in a Metal–Organic Framework Using Direct Incipient Wetness Impregnation

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Composite materials have garnered attention due to their hybrid nature, often retaining advantageous properties of parent materials. Metal–organic frameworks (MOFs) are a class of porous materials exhibiting large surface areas and high tunability. The incorporation of ruthenium nanoparticles (RuNPs) in MOFs has been achieved using bottom-up methods that involve the encapsulation of Ru(III) precursors in the MOF pores followed by hydrogenation, sometimes called incipient wetness impregnation (IWI). However, the encapsulation of RuNPs within MOF pores has never been achieved through the direct embedding of pre- synthesized RuNPs into a MOF. This work introduces a novel method for embedding RuNPs using direct incipient wetness impregnation (DIWI), a modification of traditional IWI. 1.5-nm RuNPs can be embedded into the pores of MOF-808 using DIWI in a well-dispersed egg-yolk configuration.

This method shows promise for large-scale synthesis of MOF and nanoparticle composites. The obtained composite (RuNP@MOF-808) is characterized via ICP-MS, nitrogen gas adsorption, and TEM EDX, suggesting successful embedding of nanoparticles through a consistent decrease in pore volume and surface area with increasing Ru loading. These findings underscore the potential of DIWI for optimizing heterogeneous catalysts in CO_2 methanation and suggest broader implications for tailored, cost-effective modifications of MOFs for industrial applications.

Improving Carbon Dot Mediated Drug Delivery Via Drug Conjugation Through Dynamic Imine Bonds Using Mechanochemistry: A Novel Approach

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Over the past decade, nanomaterial-based targeted drug delivery of therapeutics has come to light. While many nanomaterials show remarkable properties, they suffer from numerous drawbacks such as poor cellular compatibility and uptake, poor water dispersibility and lack of any intrinsic trackable markers. It is in this regard that carbon dots (CDs) offer a promising alternative as they are dispersible in aqueous media, possess low cytotoxicity and exhibit intrinsic fluorescence with remarkable quantum yields. The goals of this work include (i) developing a novel functionalization strategy of therapeutic agents to the surface of CDs relying on accessible surface functional groups, (ii) investigating drug release under a stimuli responsive paradigm and (iii) evaluating in vitro cytotoxicity in living mammalian cell lines. Conjugation of nabumetone (NAB), a model therapeutic was successfully carried out utilizing mechanochemistry as a novel approach to form dynamic imine bonds. Characterization techniques such as FT-IR, ^{1}H-NMR, XPS, and XRD confirmed successful formation of the drug-CD complex. Additionally, TGA was used to confirm a drug loading capacity of 28 mg/g. Preliminary drug release experiments were carried out and it was found that the CD delivery system could release NAB by cleavage of acid labile imine bonds in weakly acidic environments.

Lanthanide-doped nanoparticles as promising persistent luminescent nanothermometers

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Temperature plays a key role in almost every physical, chemical or biological process at different scales. Because of that, the thermometer market represents around 80% of the sensor market worldwide. The most widely used thermometers are thermocouple-based systems but these are not suitable for some applications where the sample cannot be placed in contact with the thermocouple, or can be disturbed or contaminated easily. In these cases, luminescent thermometers could be an ideal alternative. Taking advantage of the thermally-coupled states of some lanthanide ions, it is possible to use ratiometric readouts to use it as a luminescent thermometer. Nevertheless, the need for constant excitation can lead to sample heating and light scattering which affects the signal to noise ratio and reduces the accuracy of the thermometer. To overcome this limitation, we are developing persistent luminescent nanothermometers to do thermometry without needing constant excitation during the temperature readout. We have synthesized different persistent luminescent materials with bright and long persistent luminescence that present the same decay profile for the thermally coupled states, paving the way for applications using these novel sensors.

Automated Synthesis of DNA Nanostructures

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McGill University

DNA nanotechnology has revolutionized our ability to position matter at the nanoscale, opening new opportunities in materials design, drug delivery and biosensing.

Inspired by the automated synthesis of peptides and DNA, our primary aim is to devise an automated assembly method for DNA nanomaterials. This method minimizes the number of distinct DNA strands essential for fabricating these highly controlled materials while maintaining their 3D structure.

In this talk, I will describe how single molecule fluorescence studies were applied to design a fully automated method to produce sequence and size-defined DNA nanotubes. The programmed positioning of - fluorescently tagged - non-covalent building elements 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, the rung docking kinetics and the yield of each addition step can be quantitatively determined. Here, intensity jumps (docking) and drops (photobleaching) are used, respectively, to establish the coupling and stoichiometry. This procedure informs the solid-phase synthetic strategy and facilitates the iterative improvement of assembly parameters, revealing differences in assembly dynamics with distance to the support surface, as the nanotube is built up from the solid support.

Thermo-responsive protein-polymer hybrid nanoparticles for drug delivery

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Currently, nano-structured controlled release systems, known as drug delivery systems, have gained attention for their ability to enhance therapeutic efficacy, while minimizing adverse effects of therapeutic agents in their free form. This work will describe design, synthesis and characterization of thermosensitive hybrid nanoparticles based on silk fibroin (SF) protein and poly(N-vinylcaprolactam) (PNVCL). The hybrid system is prepared using the grafting-from technique, with reversible addition-fragmentation chain transfer (RAFT) polymerization. We utilized the thermosensitive properties of PNVCL to develop a nanocarrier capable of delivering therapeutic agents to a target site and provide controlled release through changes in temperature. The hybrid system was characterized using FTIR, TGA, and PXRD, and subsequently utilized to prepare nanoparticles with an average size of 200 nm. Curcumin was used as a model drug to investigate the loading capacity and thermosensitive release profile of this new nanocarrier, with studies conducted at temperatures of 25°C and 40°C. Results showed higher and controlled release of curcumin at temperatures above body temperature. Cytotoxicity studies on MRC5 cells indicated that both blank nanoparticles and those loaded with curcumin did not exhibit cytotoxicity to healthy cells. The results demonstrate great potential of the developed system in the field of drug delivery.

Silver-Enhanced FLuorescence: A New Frontier to Revolutionize Cellular Imaging

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Silver nanoparticles (AgNPs) have emerged as powerful tools to enhance fluorescence in live-cell microscopy, addressing common challenges like photobleaching and phototoxicity. Live-cell fluorescence microscopy traditionally requires high energy light to achieve sufficient signal-to-noise ratios, leading to the degradation of fluorophores and damage to cellular structures. AgNPs, when exposed to light, generate surface plasmons that amplify the excitation of nearby fluorophores, significantly enhancing fluorescence emission. In our prior work, we demonstrated that AgNPs, once internalized by cells, accumulate within lysosomes and enhance the fluorescence of lysosome-targeted probes without causing cytotoxic effects. This allows for accurate tracking of lysosomal motility using lower laser power, preserving normal lysosome dynamics. Building on these findings, we hypothesize that conjugating AgNPs to lysosome-specific probes such as fluorescent dextran will further optimize fluorescence, reduce the required treatment time, and streamline the imaging process. This novel approach promises the development of a new generation of “super probes,” enabling efficient, high-resolution imaging with reduced phototoxicity and photobleaching. The successful implementation of AgNP-conjugated probes could revolutionize lysosome imaging, providing critical insights into endo-lysosomal dynamics while minimizing cellular damage.

CHEMICAL ENGINEERING

Titania Nanotube Semiconductor Arrays for Copper(I)-Bis(diimine) Sensitized Photoelectrodes.

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The use of chemical bonds to store solar energy is a way to advance current sustainability goals and address intermittent limitations. The approach of interest to drive these processes is to use a bespoke semiconductor surface implemented in a photoelectrode to absorb light and generate charge carriers that can drive redox reactions such as the direct oxidation of adsorbed species on the photoanode. To minimize the recombination of photogenerated electron-hole pairs, molecular donor-chromophore-acceptor (D-C-A) systems can be used to sensitize wide bandgap semiconductors for visible light absorption and to generate (high energy) long- living charge separated states. Presented here is a highly ordered and oriented array of TiO_2 1-dimensional nanostructure purpose-grown using a self-organizing electrochemical anodization approach (SOA) and functionalized with a Cu(I)-based chromophore. The resulting photoanode is investigated against a water oxidation catalyst (e.g., [Cp*Ir(pyalk)OH], pyalk = 2-(pyridine-2-yl)propan-2-ol) for the ability to generate oxidizing equivalents that can subsequently drive follow-on oxidation reactions.

Enhanced Fouling Resistance in Bio-Effluents Management Using Bacterial Cellulose- Graphene Oxide Composite Membranes.

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Bacterial cellulose (BC) composites are increasingly being investigated as promising renewable materials for various industrial and environmental applications. However, their applications as free-standing membranes for water decontamination remains challenging due to lower compressive strength, minimal fouling resistance, and poor selectivity. The *In-situ* incorporation of GO, a nano-filler, into the three-dimensional BC network enhances the composite's wet compressive strength and permeation properties. The BC-GO composites were synthesized using a novel *In-situ* biosynthesis method with polyethylene glycol (PEG-400) to effectively disperse GO within the culture medium. The resultant membranes underwent pressure-driven filtration tests in a cross-flow filtration setup. The BC-GO composites exhibited a sixfold increase in compressive strength, effectively preventing membrane hornification under pressure. The composite membranes demonstrated a significantly improved flux of 380 LMH and a flux recovery rate of 95%. The hydrophilic functional groups of the BC-GO membranes effectively hindered the deposition of natural organic matter (NOM), thereby enhancing flux recovery. The membranes were further evaluated for water decontamination using a bacterial broth solution containing freshly cultured *E. coli.* Flow cytometry analysis confirmed that the BC-GO composites exhibited superior anti-fouling properties compared to pristine BC membranes, resulting in enhanced removal of microbial contaminants from water.

Local characterization of phases in 3D-printed semi-crystalline polymers

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Additive manufacturing consists of depositing material robotically following cartesian movements. These movement are precalculated following a computer aided design (CAD) and give 3D printing shape and material versatility. This manufacturing technique opens a new path towards studying the structure – processing – properties relationships of polymer materials. The widespread adoption of 3D printing has given rise to new challenges, as the growing demand escalates the pace at which printers must operate.

Consequently, issues such as delamination and reduced strength in layer-to-layer adhesion have emerged. These issues carry notable significance, resulting in the production of weaker final products in terms, among others, of mechanical properties. One of the current solutions involve reducing printing speeds, although this approach is less than ideal in terms of productivity. Here, gaining a deeper understanding of polymer crystallinity kinetics and the entanglement of chains between layers provides a clearer insight into the macromolecular mechanisms governing the realm of 3D printing. To establish these relationships, a combination of differential scanning calorimetry (DSC) and spectroscopy techniques are used to monitor the crystallisation that takes place following polymer extrusion during the printing process. The work presented herein offers insights that can lead to optimized performance and versatility in AM.

Conjugated Benzoic Imine-Based Dual Acid/Light-Responsive Polymeric Nanocarriers for Enhanced Drug Delivery: Synthesis and Degradation

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Stimuli-responsive degradable amphiphilic block copolymers (SRD-ABPs) have garnered significant interest as promising building blocks for constructing advanced nanoassembliescapable of controlled release of encapsulated pharmaceuticals. Recent progress in this field has focused on the synthesis of dual-responsive SRD-ABPs, designed to respond to distinct environmental stimuli, such as pH changes and light exposure, through the incorporation of two distinct cleavable linkages. This study presents a novel strategy to achieve dual responsiveness to both acidic pH and light stimuli using a single, strategically designed labile linkage based on conjugated benzoic imine chemistry.

Our approach involved synthesizing poly(ethylene glycol)-based SRD-ABPs via reversible deactivation radical polymerization, which allowed for precise control over polymer chain length. Subsequently, we utilized post-polymerization modification to introduce conjugated benzoic imine pendants into the hydrophobic block of the copolymer, forming nanoparticles with a core-shell structure. These nanoparticles exhibited colloidal stability in aqueous environments, with a hydrophobic core that is both acid and light- responsive, surrounded by a hydrophilic corona. Following proof-of-concept studies, we extended our approach to fabricate core-crosslinked nanoassemblies with enhanced stability under physiological conditions, while maintaining the ability to rapidly degrade under stimuli.These advanced polymeric nanoassemblies demonstrate considerable potential as a targeted drug delivery platform.

Uncovering the Properties of dPGA: A Stable Alternative for Long-Term Neural Cell Culture Substrates

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Polylysine has long served as one of the primary polymer coatings for adherent cell culture. However, its susceptibility to proteolysis limits its effectiveness for stable long-term healthy cell cultures. Recently, dendritic polyglycerol amine (dPGA) has emerged as a promising alternative, especially for neural cell cultures, due to its enhanced stability against protease degradation. Although dPGA provides improved cell support, the specific properties contributing to its success remain unclear and warrant further study. Here, we present a fundamental characterization of dPGA upon surface immobilization, examining its growth and morphology after deposition on silicon wafers via ellipsometry and atomic force microscopy (AFM).

Colloidal silica was utilized as another substrate to investigate dPGA's charge via zeta potential, adsorption amount via thermogravimetric analysis (TGA), chain mobility via solid-state NMR spectroscopy and high- resolution magic angle spinning (HR-MAS).

Self-Healing Poly(Hindered Urea) Polymer Network as Coating Layer on Carbon/Sulfur Composite in High-Performance Lithium-Sulfur Batteries

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Covalent adaptive networks (CANs) have emerged as a promising platform for self-healing and reprocessability in applications like biomedical devices, electronics, and coatings. Typical dynamic CANs integrated with disulfide, imine, and boronic ester, hindered urea bond (HUB) undergoes reversible exchange under catalyst-free conditions and mild temperatures. Recently, we have explored dynamic hindered urea chemistry to develop robust a poly(hindered urea) (PHU) network to enhance the performance of lithium- sulfur (Li-S) batteries. These batteries face challenges such as polysulfide shuttling, slow redox kinetics, and volume expansion.

This presentation describes the two-step fabrication of a self-healable PHU crosslinked with HUBs through step-growth polymerization, including the preparation of a pre-polyurea consisting of hexamethylene diisocyanate and poly(dimethylsiloxane) diamine, followed by the addition reaction of a tetra-functional secondary amine with bulky t-butylamino group as a dynamic crosslinker. The fabricated PHU was proven to be homogenous and possessed excellent thermal stability and mechanical properties. Being formulated with C/S composite, the self-healable sulfur cathode as PHU@C/S cathodes exhibit favorable cycle stability and maintenance of capacity retention.This work illustrates a straightforward approach to designing polymeric networks for electrochemical applications as a promising strategy for the development of high-performance Li-S batteries and advanced HUB-based materials with excellent self-healing and reprocessability.

Preparation and characterization of polymer:photosensitizer blends.

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The functionalization of the surface of a 3D object enables access to various interesting properties, such as photodynamic inactivation (PDI). PDI is a method for eliminating bacteria and viruses by using singlet oxygen as a cytotoxic element produced with a photosensitizer. Our project is based on the hypothesis of incorporating this photosensitizer into the 3D object (i.e., in the formulation used for printing) instead of functionalizing the surface of the already printed object. Herein, we explore the correlation between the shape, and properties of a material in terms of singlet oxygen production by printing a thermoset polymer, such as PDMS containing photosensitizers such as methylene blue. The blend is printed using direct-ink writing (DIW). First, the rheological properties of the formulation are studied to achieve a better understanding of the crosslinking of the thermoset. Additionally, profilometry measurements have been used to characterize the print fidelity of the 3D printed samples. Second, the apparent rate of singlet oxygen production is indirectly evaluated to assess the impact of different surface-to-volume ratio of the 3D printed samples. These results help us to rationally design 3D printed architectures with optimal surface-to-volume ratio that could be useful in the context of PDI.

Abstracts – Poster Presentations

ANALYTICAL CHEMISTRY

Screening of Reactive Metabolites by LC-MS/MS Using Different Trapping Agents and Isotopic Labeling

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The human body is exposed to a variety of endogenous and exogenous substances, which can become toxic through the formation of reactive metabolites. To mitigate their harmful effects, phases I and II of metabolism involve reactions that increase the solubility of metabolites, facilitating their elimination. These processes are mediated by cytochrome P450 enzymes, which play a key role in the metabolism of most xenobiotics.

Common techniques to evaluate the formation of reactive metabolites include *in vitro* trapping with glutathione (GSH) and characterization by liquid chromatography-tandem mass spectrometry (LC-MS/MS).

The aim of this study is to develop an analytical method for identifying previously uncharacterized reactive metabolites using untargeted LC-MS/MS. A series of compounds (three dyes, two endogenous hormones, and one synthetic hormone) were incubated with rat liver microsomes, with GSH and *N*-acetylcysteine (NAC) as trapping agents. Isotopic labeling with deuterated analogs was also employed for structural elucidation and to reduce false positives. The mass difference between light and heavy compounds facilitates the confirmation of metabolites and adducts, as well as the identification of metabolic sites. This approach has led to the identification of several molecules capable of forming adducts, and we will present the results of their characterization.

Optimizing Protocols for Combining Imaging Mass Spectrometry (IMS) and Optical Imaging of Traditional Histologically Stained Tissues; A Step Towards Integrating IMS into Digital Pathology.

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Imaging mass spectrometry (IMS) is a powerful analytical technique that combines mass spectrometry with imaging to map the distribution of analytes in biological samples. This study explores a workflow for multimodal tissue analysis (sequential vs consecutive) by combining IMS with optical imaging of histologically stained tissues, thereby enhancing the interpretative value of samples. Furthermore, we utilized laser-etched indium tin oxide (ITO) glass slides to improve image registration accuracy, with the aim to achieve spatial resolutions capable of single-cell analyses. Mouse brain tissues were analyzed using cluster ion beam secondary ion mass spectrometry (SIMS) and/or matrix laser desorption ionization (MALDI) mass spectrometry, with 1, 5-diaminonaphthalene matrix applied for high-resolution imaging. The resulting IMS images were overlaid with serial or post-analysis hematoxylin and eosin (H&E) stained sections. The study compared the effectiveness of image overlays using laser-etched fiducial markers on glass slides against traditional features on tissue sections. Results indicated that the fiducial markers provided significantly better alignment and accuracy. This research demonstrates the feasibility and benefits of integrating IMS with optical imaging, marking progress towards improved diagnostic capabilities in digital pathology.

INORGANIC CHEMISTRY

Co(III) amidine-N-oxide complexes exhibiting novel photophysical characteristics and relaxation pathways

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The development of photoactive transition metal complexes has traditionally focused on second- and third- row transition metal ions, such as ruthenium, iridium, and platinum, due to their favorable photophysical properties. These metals are scarce, expensive, and pose environmental concerns, prompting a shift towards first-row transition metal ions as more sustainable alternatives. First-row transition metal complexes (e.g., those based on iron, copper, cobalt, nickel, and zinc) offer several advantages, including abundance, lower cost, and reduced environmental impact. Despite these benefits, these metal complexes often exhibit less desirable photophysical characteristics, such as shorter excited-state lifetimes and lower photostability.

Overcoming these challenges through ligand design, coordination geometry optimization, and tuning electronic properties is crucial to unlocking the potential of these metals for applications in solar energy conversion, photocatalysis, and light-emitting devices. Herein, we present a novel class of Co(III)-amidine

N-oxide complexes exhibiting weak low energy LMCT absorptions beyond 500 nm. High lying p-orbitals on the ligand scaffold lead to this novel photophysical properties wherein the complexes refuse to obey Kasha and Vavilov rules. The nanosecond excited-state lifetimes of these complexes pave the way to new avenues for p-donor ligands in the enhancement of optoelectronic properties of complexes of abundant transition metal ions.

Mechanochemical Synthesis of Aminoquinones

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Concordia University

Aminoquinones constitute an important class of bioactive molecules, known for their potential as anticancer agents and their role as redox-active compounds in various biochemical pathways. The direct coupling of C(sp^2)-H and N-H bonds for C-N bond formation in these compounds presents a compelling strategy, but it is often complicated by competing radical pathways that can hinder selectivity, Conventional methods also typically involve hazardous organic solvents like dichloromethane, contributing significantly to environmental pollution. In fact, the pharmaceutical and fine-chemical industries generate large quantities of chemical waste, with approximately 80% of this waste coming from solvents.

In this context, mechanochemical methods offer a promising alternative, providing greener and more sustainable synthetic routes, while improving reaction selectivity and efficiency, all without relying on toxic volatile solvents. This presentation highlights our recent progress in developing mechanochemical iron-catalyzed aerobic coupling of *p*-quinones with secondary amines to yield 2-amino-1,4-quinone products. Additionally, we explore various mechanochemical techniques, including ball-milling, grinding, and shaking, to elucidate the influence of mechanical force on the reaction.

Furthermore, we are currently expanding this idea by investigating the efficacy of conducting these reactions in the absence of a metal catalyst. For example, using blue LED light simplifies the workup process, thereby allowing for direct application of the resultant powder. This ongoing work represents a significant step toward the development of efficient and environmentally benign methodologies for C-N bond formation.

Synthesis and characterization of AMidine OXide (AMOX) ligands with photoactive anthracene core and their associated Ni(II) complexes.

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The photophysical and structural properties of amidine oxide (AMOX) ligands and complexes make them interesting candidates as components of photosensitizers and/or catalysts, in the optics of an artificial photosynthetic system. The ligands were synthesized by *N*-oxidation of amidines containing anthracene and Br-phenyl on the central carbon by *m*-CPBA. The complexes were then formed from salts of Ni(II). Both the ligands and the complexes were characterized by NMR and UV-vis spectroscopy, and mass spectrometry.
The crystal structures of both the ligands and the complexes were also elucidated by X-ray diffraction analysis.

Hydroxylamines and Copper: Enabling Selective Redox Reactions *via* Ligand Design

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The intrinsic reactivity of arylhydroxylamines (ArNHOH) and nitrosoarenes (ArN=O) as redox intermediates, along with their biological relevance, has made them of significant interest for use as catalysts, particularly in C-N bond formation reactions. Their relatively low-lying frontier orbitals facilitate electron transfers with redox-active metals such as copper however, this pathway is difficult to control and often leads to disproportionation and a mixture of products. Recently, our group has shown that this reactivity can be thwarted by strategic ligand design as we reported the synthesis and characterization of the first examples of metastable Cu-ArNHOH complexes. As anticipated, these complexes were able to catalyze two-electron aerobic oxidations of alcohols via the one-electron Cu(I/II) shuttle. In this context, the arylnitrosyl radical ($ArNO^{\bullet-}$), as the highly reactive one-electron intermediate, is of particular interest for investigating the complex redox chemistry between the arylhydroxylamine and copper ions.
Herein, we present a pentadentate ligand bearing an ArNHOH function which, upon complexation with copper, is selectively oxidized to a stable arylnitrosyl radical. This complex has been thoroughly characterized by an array of crystallographic, magnetic, electrochemical, spectroscopic, and theoretical methods to decipher the electronic structure. Furthermore, we investigated the reactivity of the ArNHOH under a variety of condtions.

First row transition metal complexes as affordable and abundant photosensitizers to replace precious metal complexes.

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There is a great need to replace precious metals in photochemical reactions. In this regard we prepared room-temperature luminescent $Co^{III}(dGPy)_2(X)_3$ (dGPy = 2,6-bis(1,5,7-triazabicyclo[4.4.0]dec-5-ene)pyridine, X = BF_4^- or PF_6^-) complexes that show LMCT (Ligand to Metal Charge Transfer) and LLCT (Ligand to Ligand Charge Transfer) transitions in the relatively low-energy UV region (λ_{abs}≈360–400 nm) and quasi-reversible reductions ($E^{1/2(red)}$= −0.58 V vs. SCE) in their electrochemistry. A blue emission from the excited state of$Co^{III}(dGPy)_2(X)_3$ can be linked to the large bite angle and strong ???? donation of the guanidine moieties. The combination of these effects helps separate the emissive ^{3}LMCT state and the non-emissive ^{3}MC state. Herein we present a new photoredox catalyst for the regioselective mono trifluoromethylation of polyarene but also for the photosynthesis of H_2.

Controlled Synthesis of Novel Twinned MOF-199 via Reaction-Diffusion Framework In Hydrogel

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During crystal growth, variations in stress or temperature can lead to the formation of two or more intergrown crystals with different orientations, a phenomenon known as twinning. Twinning can significantly alter the electrical, mechanical, and optical properties of crystal. Twinning in metal-organic frameworks (MOFs) has been observed in few systems, however controlling this phenomenon remains challenging. Herein, we report the successful synthesis and precise control of novel twinned MOF-199 crystals, exhibiting space group Pa*3*, within a hydrogel using reaction-diffusion frameworks. Our study reveals a compelling relationship between the degree of supersaturation and the twinning behavior of MOF-199, elucidating the transition from twinned to untwinned structures as the distance from the interface increases. We also identify a rare twin law of [-100, 001, 010], facilitating the formation of the space group Pa*3*, distinct from the more common Fm3m.

Molecular Copper(I)-Sensitized Photoanodes for Alcohol Oxidation under Ambient Conditions

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Dye-sensitized photoelectrochemical cells can enable the production of molecules currently accessible through energetically demanding syntheses. Copper(I)-based dyes represent electronically tunable charge transfer and separation systems that can be utilized in such transformations. In this presentation, we explore a Cu(I)-bisdiimine donor-chromophore-acceptor dye with an absorbance in the visible part of the solar spectrum composed of a phenothiazine electron donor, and dipyrido[3,2-*a*:2′,3′-*c*]phenazine electron acceptor. This complex is incorporated onto a zinc oxide nanowire semiconductor surface effectively forming a photoanode that is characterized spectroscopically and electrochemically. We investigate the photo- oxidation of hydroquinone, and the photosensitization of 2,2,6,6-tetramethylpiperidine-1-oxyl and N- hydroxyphthalimide for the oxidation of furfuryl alcohol to furfuraldehyde, resulting in near quantitative conversions, with poor selectivity to the alcohol. This opens the door to a non-selective heterogeneous sensitizer, capable of sensitizing or photocatalyzing a variety of oxidation reactions, provided there is appropriate redox leveling.

Non-Random Chiral Crystallization of Epsomite

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In 1848, Louis Pasteur was able to separate two distinct enantiomorphic (right- and left-handed) crystals of sodium ammonium tartrate tetrahydrate by visual inspection of their crystal morphology. Epsomite ($MgSO_4 \cdot 7H_2O$), also known as Epsom salt, is a chiral (handed) sulfate mineral composed of achiral (non- handed) building blocks. Epsomite crystals can also be separated according to their distinguishable mirror- image morphologies where, upon crystallization one expects an equal population of left- and right-handed crystals. This project focuses on determining the handedness of epsomite crystals through crystal morphologyanalysis and the use of chiral etch pits on crystal faces. Surprisingly, the crystallization of epsomite favours the left-handed form, which is believed to be due to the presence of hidden handedness in the environment.

PHYSICAL CHEMISTRY

Chiral Induced Spin Selectivity in Triboelectric Nanogenerators

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Contact electrification (CE) or triboelectrification, is a phenomenon by which electric charges move between dissimilar materials upon contact. Contact electrification for spin-selective electron transfer has only recently been explored at the liquid-solid interface of different liquids and ferrimagnetic solids under a magnetic field. Another method for spin-selective electron transfer relies on using chiral molecules as spin filters through the chiral induced spin selectivity (CISS) effect. Herein, we have designed and built a triboelectric nanogenerator (TENG) to investigate the CISS effect during contact electrification. To this end, we demonstrate contact separation TENG devices that generate stable and reproducible electrical output, where we have monitored the voltage and current under various spin filter conditions. The device's mechanical motion is provided by a piston controlled by a pneumatic control system for low-frequency or an electromechanical vibrator system for high-frequency contact separation. Specifically, we have prepared ferromagnetic Ni-coated substrates functionalized with chiral hybrid organic-inorganic perovskites. (HOIPs; (Rmethylbenzylammonium)2CuCl4 and (S-methylbenzylammonium)2CuCl4) These materials have shown high spin polarization, good stability, facile syntheses, and preparation. This has made them an ideal candidate for this fundamental study of combining CISS and TENG.

An investigation of CO2 laser pattern creation on Polydimethylsiloxane thin film surface in daytime passive radiative cooling

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Passive daytime radiate cooling (PDRC) has been driving people’s attention in recent years, which aims to let objects radiate energy to the cooler outer space and cool down without any energy input during direct sunlight. It takes advantage of certain materials with strong absorption and emission at the atmospheric transparent window, where the atmosphere has minimal absorption to the energy emitted at 8-13 μm. With these kinds of materials covered on the building, the building can cool down during the daytime.

Polydimethylsiloxane (PDMS) has a strong emission at the atmospheric transparent window, and creating micron-meter scale patterns on the PDMS surface can enhance the emissivity even more. However, the creation of the patterns needs non-green solvents and mold, and a large amount of waste can be produced if massive production of patterned PDMS film is needed. Here we proposed a potential mold-free and solvent- free pattern creation method, by sending a CO2 laser at an appropriate intensity to an uncured PDMS surface, and the surface responds to having a self-forming pattern We are also able to selectively cure PDMS thin film by manipulating the laser intensity and distance between the laser and the film.

Impact of Antibacterial Cysteine-Derived Carbon Dots on the Biophysical Properties of Pulmonary Surfactant

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One of the most common types of pulmonary infection diseases is bacterial pneumonia which can cause mild to life-threatening illness in people of all ages. Presently, antibiotics are used as first-line drugs to treatpneumonia. Due to the limitations of systemic administration methods, inhalation, as a targeted administration route, can deliver the drug directly to infected cells. [1] Inhaled nebulized nanomedicines (NMs) are gaining attention among researchers due to being transported into the deep lung deposition at the alveoli region. However, the pulmonary fate of inhaled NMs is affected by the bio-nano interactions with pulmonary surfactant (PS) at the air/alveoli fluid interface, which alters the fate of inhaled therapeutic NMs and the lung's physiological function. Since the role of PS is reducing the surface tension at the air/alveoli interface to ease the breathing process, whatever affects the standard functionality of PS could cause respiratory problems. Therefore, the interaction of NMs with PS can cause changing surface tension, PS phase structure, and reservoir formation. The consequences of each alteration have a diverse impact on the breathing system. [2] Recently, the antibacterial cysteine-derived carbon dots (cys-CDs) have been successfully developed [3]. Antibacterial properties of these cys-CDs against different strains of bacteria show promising results toward generating new ideas in the field of antibiotics. In this research project, the effects of different concentrations of antibacterial cys-CDs on the phase behavior and lateral structure of lung surfactant binary mixture model (DPPC: POPG) were investigated at the air/water interface using surface pressure−area isotherms and Brewster angle microscopy, respectively. Additionally, atomic force microscopy was used to image the morphology of films transferred onto a mica substrate with nanometer resolution. The results revealed that the presence of cys-CDs resulted in hindering lipid packing and loss of material resulting in shifts to higher molecular area during early compression for monolayer isotherms. However, further studies are aimed at looking over the more complex lung lining memetics.

ORGANIC CHEMISTRY

Drug Design, Synthesis and Structure-Activity-Relationship Studies of 1,3,5-Triazine Derivatives as Positive Allosteric Modulators for G-Protein-Coupled Receptor 68 (GPR- 68)

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G-protein-coupled receptors are the largest family of proteins encoded in the genome, which transduce signals for the most diverse ligands of any receptor family. Among these, many GPRs are understudied or "dark receptors", whose physiological roles are unknown. One of these is GPR-68, a transmembrane receptor that can induce physiological effects when activated by protons. One of these known effects is to induce the release of calcium, which may promote stem cell differentiation, making GPR-68 an attractive target for drug development.

Molecular Modelling studies proposed that 1,3,5-triazine scaffold have strong affinity for the GPR-68, being therefore considered the pharmacophore group. Among many candidates tested against this receptor, Ogerin, a trisubstituted form of this molecule, showed a promising biological activity, behaving as Positive Allosteric Modulator (PAM).

In this work, different Drug-Design strategies were employed for the synthesis of new 1,3,5-triazine derivatives, and the resulting calcium release was assessed.The resulting Structure-Activity-Relationship (SAR) studies may be used to assess possible other pharmacophores for GPR-68. Different synthetic routes were developed to produce new 1,3,5-triazines derivatives as novel modulators of G-protein-coupled receptor 68.

Synthesis and enantioselective reduction of prochiral α-CF_3 and α-SF_5 ketones

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Laval University

As the demand for both fluoro-pharmaceuticals and single enantiomer drugs increases, there is a need for enantioselective synthetic methods towards chiral fluorinated molecules. Fluorinated groups such as trifluoromethyl (CF_3) and pentafluorosulfanyl (SF_5) bear the hallmark high electronegativity and lipophilicity of fluorinated substituents, while their distinct steric properties make them desirable bioisosteric replacements for numerous functional groups.

Due to the synthetic challenges to access pentafluorosulfanylated compounds, it is our goal to develop methodology for (1) the expedited synthesis of prochiral α-SF_5 ketones and (2) the enantioselective reduction of these ketones to chiral β-SF_5 alcohols, with an analogous method for β-CF_3 alcohols.

Our previous synthesis of α-SF_5 ketones involved the radical addition of SF_5Cl to a terminal alkyne, followed by an elimination reaction to produce the SF_5-alkyne. Subsequent gold catalysed hydration afforded the α-SF_5 ketone. We will discuss the development of a concise synthesis of α-SF_5 ketones through radical addition of SF_5Cl to enol acetates.

With these α-SF_5 ketones in hand, we sought to valorize these substrates as a gateway to a new chiral library of SF_5 compounds. After testing various reduction methods, the Noyori asymmetric transfer hydrogenation afforded high enantioselectivity and yields across a scope of aromatic α-SF_5 and α-CF_3 substrates.

Influence of Fluorine on Sterically Controlled Rhenium-catalyzed Hydroxyl Transposition to Access Enantioenriched Quaternary Centers

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The *p*-Menthylaldehyde, developed by Prof. Spino's group, is a chiral auxiliary allowing efficient access to enantioenriched tertiary centers. However, when aiming at quaternary centers, this auxiliary leads to a problematic formation of an allylic carbocation during the rhenium(VII) rearrangement of allylic alcohol, destroying its precious stereogenic information. We hypothesized that a source of fluorine, either on the chiral auxiliary or on the substrate, would prevent the formation of the allylic carbocation during the rearrangement, allowing access to enantioenriched quaternary centers. We successfully reached a quaternary center precursor through a trans-methylboration followed by its proto-demetalation and are currently optimizing the reaction conditions to test our research hypothesis.

Pantothenamide-mimicking compounds as novel antimicrobial agents

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Antimicrobial resistance (AMR) occurs when bacteria, fungi or parasites no longer respond to our medicines. AMR is an ever-growing global health crisis with a projected yearly death toll of 10 million lives in 2050.

Antimicrobial drugs with novel modes of actions are urgently required to combat these drug-resistant microbes. Pantothenamides are a promising class of compounds that display a novel mechanism of antibacterial and antiplasmodial activities. In microorganisms, these molecules can selectively transform into their CoA derivatives, before inhibiting CoA utilization. Such a multi-target mode of action is highly desired due to an expected slower onset of resistance. Yet, these compounds are hydrolyzed by pantetheinases in the blood, rendering them inactive and inadequate as clinical candidates. We have modified these pantothenamides to prevent the hydrolysis of the labile amide bond, while still allowing them to retain their potency. These pantothenamide-mimics have been modified in one of three ways: at the gem-dimethyl position, at the β-alanine linker, and by replacing the amide bond with a bioisostere. Several of the synthesised compounds display activity at low micromolar concentration towards bacteria and/or at nanomolar concentration against the malaria parasite, while being stable in blood as well as being non-toxic to human cells.

Photostable open-shelled fluorophores for near-infrared organic light-emitting diodes: a proof of concept

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Closed-shell organic materials that emit in the visible have been widely investigated in the last decades. In this context, near-infrared organic light-emitting diodes (NIR OLEDs) hold significant interest owing to their extensive applicability across various technological domains such as biosensing, optical imaging, photodynamic therapy, and ensuring security in personal identification and surveillance systems.

Because of their spin-allowed radiative decay, singlet excitons are of interest for emitting applications. Hence, the internal quantum efficiency (IQE) of closed-shell emitters is limited to 25% as dictated by spin statistics.

Radicals are open-shell molecules. They consist of an unpaired electron located on the SOMO. Owing to this, their ground and lowest excited states have a doublet multiplicity. Thus, upon electrical and optical excitation doublet excited states radiatively decay to the ground state. This opens the possibility of achieving an IQE of 100%. Within the context of NIR OLEDs, replacing traditionally used closed-shell molecules with thin films of neutral radicals is advantageous. In this work, we detail the synthesis of novel photostable radical fluorophores with a covalently attached electron-rich core and a carbon-centered organic radical. We will also present preliminary results regarding the potential application of these materials as emitters for NIR OLEDs.

The Development of Anillin-Specific Inhibitors for Treatment Against Hepatocellular Carcinoma

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Cancer is defined by an overexpression of cell-growth regulators. Cytokinesis is a well conserved process which occurs at the final stage of mitosis. Understanding the intricate relationship between cytokinesis and cancer is essential for developing targeted therapeutic strategies in order to mitigate uncontrolled cancer cell proliferation. Anillin, a key actin-binding protein, is considered to be one of the crucial regulators in cytokinesis. Considering the amino acids in Anillin involved in the cytoskeletal dynamics, specific inhibitors can be designed to disrupt its functions. As Anillin is upregulated in cancer cells, developing an Anillin-specific inhibitor provides exceptional therapeutic potential for the treatment of cancer. The objective of this project is to develop inhibitors that specifically block Anillin function. The RBD-RhoA and RBD-C2 interfaces in Anillin were identified as having key amino acids facing outward from two alpha helices. Helical motifs are known to project residues i, i+4 and i+7 on the same face of the alpha-helix. Previous research on alpha-helical mimetic compounds suggest terphenyl compounds can mimic the i, i+4 and i+7 side chains. Considering this, a library of arene and heteroarene-based terphenyl scaffolds with functional groups that can interact with the respective residues on the ANLN-RhoA binding interface was synthesized. The compounds were synthesized by optimizing cross-coupling techniques previously employed, as well as various derivatization reactions to ultimately expand the library of compounds. Structure-activity-relationship studies were implemented following *in vitro* testing by the collaborator, providing further insight into the key functional groups required to disrupt the function of Anillin.

MOLECULAR BIOLOGY

Uncovering the Protein Sorting Machinery of the Intralumenal Fragment Pathway for Membrane Remodelling

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Lysosomes play a crucial role in cellular health by degrading damaged organelles, pathogens, and unneeded proteins through pathways like endocytosis and autophagy, converting them into essential nutrients. This process depends on continuous membrane remodeling, enabling lysosomes to adapt to the cell's changing demands. Proper functioning of lysosomes relies on effective protein sorting and degradation, which are facilitated by pathways such as the Intralumenal Fragment (ILF) pathway. This pathway selectively sorts proteins for degradation, although the precise mechanism governing this process remains unclear.

Preliminary data indicate that the HOPS (Homotypic Fusion and Vacuole Protein Sorting) complex, potentially through ubiquitin binding, may mediate this sorting by selectively directing certain proteins for degradation. This project aims to uncover the molecular mechanisms that govern protein sorting within the ILF pathway. Using the model organism *S. cerevisiae*, I will tag Fet5, an iron oxidase protein degraded by this pathway, with MiniTurboID, a promiscuous biotin ligase, to capture protein interactions during sorting and identify them by mass spectrometry. This study will provide insights into lysosomal membrane remodelling, and may reveal how disruptions in this process contribute to cellular health, aging, and disease.

An Automated Approach to Streamline EV tag Discovery in Yeast.

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Extracellular Vesicles (EVs) drive intercellular communication between cells and are being leveraged as nanocarriers for drug therapies. Most researchers in the EV field produce EVs using human mesenchymal stem cells, a platform that has many limitations including cargo loading and thus slowing progress toward clinical use. To overcome related barriers, our lab has instead begun using *S. cerevisiae* – a powerhouse organism in biomanufacturing – to develop, test and produce engineered EVs for therapeutic

applications. My research goal is to design, build and test new strategies to efficiently load DNAs, RNAs and proteins into extracellular vesicles (EVs) within baker's yeast (S. cerevisiae) using methods rooted in synthetic biology. To achieve this, my project will focus on our first objective by selecting 96 candidate ExoTags based on criteria devised by our lab's previous yeast EV proteomics data. I will evaluate the EV- sorting potential of each ExoTag candidate by assembling the ExoTag sequences into a complete expression construct that includes a bioluminescence enzyme, luciferase, using Gateway cloning.

Small RNA and Freeze Survival: The Cryoprotective Functions of MicroRNA in the Frozen Muscle Tissue of The Grey Tree Frog

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The grey tree frog, *Dryophytes versicolor*, survives whole-body freezing for weeks during cold winter months. Survival in a state devoid of available food, water, or oxygen forces a reliance on metabolic rate depression (MRD) and the reprioritization of bodily functions. This study utilizes next-generation sequencing (NGS) and bioinformatic analyses to characterize changes in the microRNAome of *D. versicolor*. When comparing control to frozen groups, five microRNAs (miRNA) were found to be differentially regulated (miR-143-3p, miR-30e-3p, miR-10a-5p, miR-140-3p, and miR-148a-3p), suggesting that they play key roles in freeze survival. The KEGG and GO analyses of these changes predicted a significant negative enrichment of terms associated with cell proliferation and active metabolism while simultaneously predicting the upregulation of cell signalling terms. These results suggest a fast-acting regulatory role for miRNA in contributing to the reorganization of gene expression and the limitation of energy-expensive processes during MRD in the hind leg skeletal muscle of the frog.

Histone Arginine Methylation in the Wood Frog, *Rana sylvatica*

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The climate of the regions where the wood frog, *Rana sylvatica*, resides in causes many challenges for the animal. One of those challenges being the lack of oxygen when the frog is frozen. These frogs display various strategies and mechanisms that allow them to survive such extended periods of oxygen deprivation. Histone arginine methylation is one mechanism that these frogs use to protect themselves against anoxia.Immunoblotting was used to measure relative protein levels of various arginine methylation proteins (PRMTs) and histone marks in the wood frog brain. It was then determined that these proteins were differentially regulated when control and 24 h anoxia groups were compared with PRMT3, PRMT4, PRTM5, and PRMT7 showing singificant upregulation.

Expressing the human proteome in Saccharomyces cerevisiae as a model for advancing extracellular vesicle biology

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We combine synthetic and systems biology with *Saccharomyces cerevisiae* to study conserved proteins in extracellular vesicle (EV) biology. This work aims to build a high-throughput pipeline to express and identify human proteins in yeast EVs. Our high-throughput method expresses over 15,000 human proteins, tagged with GFP, in yeast. Using 18 gene pools and Gateway cloning, we create humanized yeast strains. Cloning efficiency is validated with Oxford nanopore sequencing, and protein expression confirmed by fluorescence microscopy and Western blotting. We use mass spectrometry on immunoprecipitated yeast EV samples to identify human proteins. Nano flow cytometry (NanoFC) quantifies GFP in EVs, with Nanoparticle tracking analysis (NTA)and TEM measuring vesicle size and morphology. Positive hits are individually cloned and validated. Our proof-of-concept study shows ~99% cloning efficiency. LC MS/MS and WB confirm GFP-tagged protein expression in yeast. Fluorescence microscopy reveals subcellular localization patterns, including sites resembling EV biogenesis. NanoFCM detects GFP+ populations in small EVs (50–200 nm), validated by NTA. Proteomic analysis identifies a subset of human proteins verified in isolation. This novel pipeline enables the engineering of yeast EVs with human proteins, creating humanized yeast strains as models for studying conserved EV protein functions in biogenesis and cellular interactions.

BIOCHEMISTRY

Impact de la SUMOylation sur les interactions de MeCP2 : Vers de nouvelles perspectives thérapeutiques pour le syndrome de Rett

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Le syndrome de Rett est une maladie neurologique rare, caractérisée par une régression progressive des capacités motrices et de communication après une phase de développement normal. Cette pathologie est principalement due à des mutations du gène MECP2, crucial pour la régulation épigénétique neuronale. La protéine MeCP2 subit un processus de modification post-traductionnelle appelée SUMOylation, où une protéine SUMO est attachée de manière covalente à une lysine de MeCP2. Ce mécanisme pourrait potentiellement renforcer ses interactions avec d'autres protéines telles que IMA3, HDAC1 et DNMT3A. Nous posons l'hypothèse que la SUMOylation augmente l'affinité de MeCP2 pour ces protéines, affectant ainsi ses fonctions dans le contexte du syndrome de Rett. Pour tester cette hypothèse, nous produirons de manière recombinante les protéines IMA3, HDAC1 et DNMT3A, et effectuerons la SUMOylation de MeCP2. Nous utiliserons la technique GST-Pull Down pour comparer les interactions entre les formes sumoylées et non-sumoylées de MeCP2 avec ses partenaires protéiques. Cette étude vise à clarifier le rôle de la SUMOylation dans les interactions protéiques, avec l'objectif de contribuer à l'amélioration des options thérapeutiques pour le syndrome de Rett. À l'avenir, l'utilisation de variants pathologiques de MeCP2 pourrait déterminer si la SUMOylation compense la perte d'interactions causée par les mutations.

Reprogramming DNA with a Small Molecule

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Nature elegantly demonstrates that structure informs function. By harnessing this inspiration and creating new structures from DNA, we can construct materials with state-of-the-art functions. In fact, it is now possible to create new nucleic acid structures via the synthetic incorporation of artificial nucleobases into the DNA sequence. However, the problem with this approach lies in the expensive and laborious techniques required for the covalent modification of DNA's backbone. To circumvent these challenges, the Sleiman group has exemplified that the addition of small molecule nucleobase-mimics induces the formation of unique nucleic acid structures. We have now discovered that poly(adenine) assembles into a new structure upon the addition of the small molecule, xanthine. This purine-based molecule was chosen because it is non- toxic, has two hydrogen bonding faces and is neutral at physiological conditions. The structure, physical properties and applications of this new DNA structure will be presented. The goal of this project is to diversify the range of available architectures in DNA nanotechnology and consequently expand the scope of applications. At the forefront of this research is the mastery of DNA; it's now possible to expand the way we think about the supramolecular polymer and harness its powers to create novel structures.

Investigating the enzymes of a novel pathway to treat bacterial infections

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The rise of antimicrobial resistance demands new strategies to combat bacterial infections. Our research focuses on developing molecules that re-sensitize highly resistant bacteria, like Salmonella enterica and Mycobacterium tuberculosis, to the human immune system. Macrophages, immune cells that engulf bacteria, release toxic molecules like itaconate to kill pathogens. However, these bacteria have adapted, using a three- enzyme itaconate degradation pathway to survive within macrophages by metabolizing itaconate as a nutrient. This pathway is poorly understood, and none of its enzymes have been characterized to date. By elucidating the mechanisms of these enzymes through kinetic and mechanistic assays, we aim to design inhibitors that block bacterial survival within macrophages. Our findings could guide the development of novel treatments that restore immune efficacy and potentially reduce the onset of antimicrobial resistance in these pathogens.

Investigating the Efficacy of Novel Peptides in combination with β-lactam antibiotics against the TEM1 β-lactamase

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β-lactams are one of the most widely prescribed classes of antibiotics in the world. Bacteria have evolved several mechanisms to counteract these antibiotics including through inactivation of the drug via the production of β-lactamases. Over the years, there have been a number of efforts to counteract β-lactamase activity through design of β-lactamase inhibitors. Such inhibitors work synergistically with β-lactams to regain susceptibility of bacteria to the β-lactam. Despite β-lactam/β-lactam inhibitor combinations being relatively new, bacteria have already evolved mechanisms of resistance to them. Thus, to keep up with this continuously evolving arms race, novel antimicrobials are needed. Previously, our lab has designed novel 14- mer peptides which have been proven to bind allosterically to the TEM-1 β-lactamase and significantly decrease TEM-1 action. Currently, we are performing checkerboard assays to investigate if our novel peptides and the β-lactam, ampicillin, produce a synergistic effect in vivo. Our aim is to further improve the specificity and efficacy of these peptides and investigate their safety for human antimicrobial use.

Defining the functional properties of cyclopropane fatty acid synthase from Pseudomonas aeruginosa

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The emergence of antibiotic-resistant bacteria poses a significant threat to global health, necessitating research into new antibiotics. A major challenge in this regard is the bacterial membrane, which protects bacteria from environmental stress and antibiotics. Understanding the biogenesis and structure of bacterial membranes is critical for the development of novel drugs. Gram-negative bacteria, including Pseudomonas aeruginosa (PA), modify their membrane lipid composition under stress to enhance survival. One such modification is the biosynthesis of cyclopropane fatty acids (CFAs), which accumulate during stationary phase or under stress and contribute to membrane stability, resistance, and virulence. The objective of this research is to elucidate the mechanisms of CFA biosynthesis in PA. A reverse-phase liquid chromatography- mass spectrometry method was developed to profile changes in the PA lipidome, revealing an increase in CFA production during stationary phase. In contrast, genetic deletion of the enzyme responsible for CFA biosynthesis (CFA synthase) abrogated CFA production. The purified PA-CFAS enzyme forms a stable homodimer and shows a kinetic preference for phosphatidylglycerol lipid substrates and membranes enriched with unsaturated acyl chains. A bioinformatic analysis revealed divergent amino acid sequences in the lipid binding domain of CFAS, suggesting distinct membrane-binding properties among orthologues.

Unraveling Lanthipeptide Biosynthesis: High-Resolution Insights via Nuclear Magnetic Resonance.

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HalM2 is a model class II lanthipeptide biosynthetic enzyme, catalyzing post-translational modifications of the HalA2 precursor peptide. It recognizes the *N*-terminal leader peptide portion of the precursor and facilitates the dehydration of seven serine/threonine residues and the formation of four thioether rings in the *C*-terminal core peptide with high fidelity, yielding a single poly-macrocyclic isomer. Despite extensive study, the fidelity source remains unknown, necessitating high-resolution NMR techniques. The enzyme kinetics will be studied at an atomic level via a time-resolved HSQC-NMR experiment where a ^{13}C labeled HalA2 is incubated with HalM2 and $^{13}C/^{1}H$ correlation spectra are collected over 24 hours. Changes in peak intensities will provide kinetic information on each HalA2 dehydration and cyclization event. This approach offers details about timing of the post-translational modifications and high-resolution insight into the regio- and stereochemistry of the thioether bridges. We will also employ saturation transfer difference (STD)-NMR to identify HalA2 peptide residues crucial for enzyme recognition and probe the putative extended peptide binding site using a variety of HalM2 variant enzymes. These NMR approaches will provide the first atomic- level details to the complex, multistep maturation of an antimicrobial lanthipeptide opening the door for rational manipulation of the system through targeted binding interactions.

Assembly of MacAB-TolC, a multidrug efflux pump, and its role in antimicrobial resistance

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Antimicrobial resistance is a global health phenomenon as bacteria are continuously finding new ways to develop resistance to antibiotics. One method of resistance is the use of multidrug efflux pumps that transport antibiotics out of the bacterial cell. MacAB-TolC, a member of the ATP-binding cassette (ABC) superfamily, is a tripartite multidrug efflux pump that is found in Gram-negative bacteria. It is implicated in tigecycline and colistin resistance, along with biofilm formation, in the critical priority pathogen A. baumannii.

Additionally, MacAB-TolC has a stoichiometry of 6:2:3 (MacA : MacB : TolC). Due to its complexity, the assembly of this efflux pump is likely regulated in bacteria, but the mechanism is poorly understood. This project develops a fluorescence-based approach to monitor the binding of MacAB and begins to characterize this mechanism of assembly by reconstituting these proteins into lipid bilayers. Understanding the mechanism of MacAB-TolC assembly and its regulation would not only provide insight into developing a strategy that could be applied to other tripartite efflux pumps but could also aid in the design of small molecule inhibitors, which would help in the fight against antimicrobial resistance.

An enzymatic pathway for [18F] FDG synthesis on a microfluidic platform.

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The [^18F]FDG (fluorodeoxyglucose) radiotracer is widely used as a molecular probe for clinical positron emission tomography (PET) imaging, primarily for cancer diagnosis, detection, and staging. However, the widespread adoption of PET technology in Canada and globally is hindered by the limited availability of FDG radiotracers, mainly due to challenges in FDG synthesis for clinical use. This synthesis requires specialized radiochemistry laboratories, which involve high startup, operating, and maintenance costs for the chemical synthesis and purification of tracers.

To address these limitations, we propose a biosynthetic approach to produce FDG using an engineered fluorinase enzyme in a microfluidic platform. A library of enzyme variants will be generated using site saturation mutagenesis. Through fluorescence detection in a high-throughput droplet microfluidic sorter, the most promising variants will be selected and characterized to produce FDG with high efficiency and selectivity.

The proposed enzymatic approach addresses several limitations of the current [^18F]FDG synthesis process. This one-step, one-pot method reduces complexity, shortens reaction times, and simplifies purification. These advancements offer a substantial advantage for PET facilities, significantly enhancing their capacity to produce FDG independently and improving access to critical diagnostic tools.

Étude de l’importance des motifs d'interaction à SUMO (SIMs) dans le mécanisme de SUMOylation et leur utilisation pour la conception de nouvelles SUMO E3 ligases synthétiques pour des applications biotechnologiques.

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La SUMOylation est une modification post-traductionnelle essentielle qui régule diverses fonctions cellulaires, notamment la stabilité et les interactions des protéines. Les SUMO E3 ligases jouent un rôle crucial dans ce processus en facilitant la conjugaison des protéines SUMO à leurs cibles spécifiques via des SIMs, modulant ainsi des milliers de protéines humaines impliquées dans des processus biologiques clés.

L’objectif est de comprendre comment les SIMs influencent l'efficacité de la SUMOylation et d'exploiter cette connaissance pour concevoir des E3 ligases synthétiques optimisées, capables de stabiliser des protéines d’intérêts. Le projet propose deux approches : un criblage à haut débit de SUMO E3 ligases avec des SIMs randomisés, et un criblage basé sur l'expression de ces ligases à la surface des bactéries pour évaluer l'efficacité de la SUMOylation. Des tests biophysiques et des modélisations structurelles via AlphaFold seront également réalisés afin d’analyser les interactions moléculaires des SUMO E3 ligases susceptible de promouvoir la SUMOylation efficacement. Ce projet permettra d’approfondir notre compréhension des processus de SUMOylation, encore peu étudiés et consolidera les connaissances mécanistiques sur les SUMO E3 ligases. La mise au point de ces modules E3 ligases permettant de stabiliser des protéines cibles ouvrira également la porte à de nouvelles applications biotechnologiques.

Characterisation of the interactome of Cytohesins, a family of ARF-GEFs, in ARF signaling and in the regulation of focal adhesions.

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The ADP-Ribosylation Factor (ARF) proteins are small GTPases involved in membrane trafficking and cell migration, cycling between an active GTP-bound state and inactive GDP-bound state. The activation process is rate-limited by binding of GTP and the release of GDP is mediated by Guanine nucleotide Exchange Factors (GEFs). In humans, 15 GEFs are identified based on the presence of Sec7 domain which includes cytohesin (CYTH) subfamily, CYTH1-4. They are implicated in cell migration, protein trafficking and cytoskeletal modulation by activating specific ARFs. However, the interactors and mechanism governing cell migration regulation by CYTHs remains unexplored. Currently, we conducted proximity-dependent biotin identification (BioID) on the CYTH 1-4 in HeLa cells, identifying approximately 300 high confidence proximity interactors, some of it associated with focal adhesion modulation. Notably, a CYTH inhibitor, SecinH3, caused enlargement of focal adhesions in HeLa cells. Simultaneously, overexpression of CYTH3 and 4, but not CYTH1 and 2, led to the dissolution of focal adhesions. This raises the question which focal adhesion components interact with CYTH3 and 4 to modulate cell adhesion and migration. An in-depth analysis of our dataset could illuminate the specific molecular complexes involved in signaling and clarify the role of the CYTH family in focal adhesion regulation.

Capturing the Conformational Dynamics that Define Lanthipeptide Synthetase Enzymatic Function using Single Molecule Fluorescence Spectroscopy

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Natural products (NP) collectively account for a large fraction of drugs used in clinical settings. These molecules often have complex structures that render their total organic synthesis challenging. Nevertheless, natural product biosynthetic enzymes routinely achieve the synthesis of these complex structures with high catalytic efficiency and biosynthetic fidelity under mild biological conditions that are safe for the environment. Understanding NP biosynthetic enzymes on a molecular mechanistic level provides a critical blueprint for the engineering of biocatalysts to support pharmaceutical development and to provide sustainable routes to industrial scale pharmaceutical production. My proposed PhD project outlines a strategy to develop complementary tools for investigating the conformational dynamics of lanthipeptide synthetases using single molecule fluorescence spectroscopy. These measurements will provide insight into the structural fluctuations and conformational heterogeneity that guide the multistep maturation of lanthipeptides in real time. These novel data will then be combined with existing biomolecular mass spectrometry-based methods pioneered by the Thibodeaux group to better understand how catalytic efficiency and biosynthetic fidelity have emerged in lanthipeptide biosynthesis through evolvable and dynamic biomolecular interactions. This knowledge will then serve as the foundation for future rational manipulation of lanthipeptide biosynthetic enzymes.

Synthesis and Characterization of DNA Tetrahedra Containing O6- Alkylene 2'- Deoxyguanosine Cross-Links for Controlled Disassembly Triggered by a DNA Repair Protein

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O6-Alkylguanine DNA alkyltransferase (AGT) is a DNA repair protein which can remove various alkyl adducts from the O6-atom of 2'-deoxyguanosine (dG) in genomic DNA. Of particular interest is the human variant of this protein (hAGT) which has demonstrated the ability to repair an array of substrates, including DNA containing butylene and heptylene intrastrand cross-links (IaCLs) connecting the O6-atoms of adjacent 2'-deoxyguanosine (dG) residues lacking a phosphodiester linkage. Three-way junction oligonucleotides (TWJ) containing these IaCL have been designed and assembled into a DNA tetrahedron (TDN) which can be dismantled by hAGT. Given the interest of the TDN as a delivery system, we have been investigating hAGT activity as an endogenous mechanism of release.

To optimize the design for efficient hAGT triggered disassembly, the effect of longer decylene and dodecylene linkers on complex stability and hAGT interaction has been investigated. This is achieved through the preparation of a dG dimer phosphoramidite via a concise synthetic approach, followed by solid- phase synthesis of TWJ oligonucleotides involving an orthogonal chain extension. Sufficient quantities of TWJ oligonucleotides have been prepared to assess TDN structure, assembly and biophysical properties. The disassembly efficiency has been assessed for all cross-link lengths and assay optimizations have been made.

Synergizing Photosensitizers and LDE Metabolism with Ferroptosis for Targeted Cell Death

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Ferroptosis, a regulated form of cell death characterized by iron-dependent lipid peroxidation, holds promise for targeted therapies in cancer and disease. Recent work has focused on exploring ferroptosis activation through novel compounds and synergistic mechanisms. Here, we investigate the effect of Dormant Photosensitizers (DoPS), a type of photosensitizers that upon irradiation by light do not produce reactive oxygen species (ROS), unless activated by a defined mechanism. We tested the efficacy of DoPS in combination with ferroptosis inducers to elucidate their influence on cell viability.

Our study validated the hypothesis that Dormant Photosensitizers (DoPS) can effectively induce ferroptosis when co-applied with established ferroptosis inducers. Through temporal analysis of cell viability, we observed a complex dynamic between cellular proliferation and mortality, suggesting the presence of potential therapeutic windows for optimized treatment strategies.

Investigating SMYD3 Oncogenic Activity by Machine Learning: Discovering Novel Substrates and Peptide-Based Inhibitors.

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SMYD3, a lysine methyltransferase, plays a critical role in regulating numerous cellular processes via the methylation of both histone and non-histone proteins. Its overexpression has been implicated in various cancers, including lung, colorectal, prostate, and hepatocellular carcinomas, highlighting its role in tumor progression and as a prognostic marker. Despite its significance in cancer, the complete biological functions of SMYD3 are not fully understood, primarily due to the limited identification of its substrates and the lack of effective, specific inhibitors.

To address these challenges, we have developed novel peptide-based inhibitors that selectively target SMYD3 methyltransferase activity. These inhibitors are used to identify new SMYD3 substrates and characterize their roles in cancer progression. By using peptide arrays to profile the human lysine methylome, we identified SMYD3-mediated methylation targets, revealing potential biological substrates. By elucidating these targets and their downstream effects, our study aims to deepen the understanding of SMYD3-mediated oncogenesis and uncover new therapeutic opportunities.

ENVIRONMENTAL CHEMISTRY

Lithium recovery characterization with Ion sieve material

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Nowadays, lithium is a critical element for the battery industries. Lithium is abundant in saline waters and could represent a sustainable supply of this element; however, the presence of high concentrations of competing ions in these waters impair its capture using adsorption processes. This study is focused on the selective lithium recovery from saline waters using an ion sieve material based on lithium titanium oxide material. The capacity for lithium adsorption was tested with commercial LTO and LTO that was delithiated to form an ion sieve structure that can differentiate between lithium and competing ions. To identify the optimal material properties for selective adsorption, different delithiated LTO materials (or HTO) were produced by exposing the commercial LTO powder to hydrochloric acid for different periods of time. These materials were characterized and then evaluated for their lithium adsorption performance to establish a relationship between delithiation degree and lithium adsorption capacity in saline waters. These results provide insights into the development of new selective adsorbents for lithium capture.

From Properties to Impacts: Environmental Modeling of Tire-Derived Chemicals

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Tires, as an integral part of modern transportation, undergo constant wear and tear, releasing a complex mixture of tire-derived chemicals (TDCs) into the environment. This release process contributes to the dispersion of TDCs across various environmental compartments, including soil, water bodies, and air, as recent monitoring work has demonstrated. However, the environmental distribution, transport mechanisms, and transformation processes of these compounds are not well understood. This is partly due to insufficient information on their physico-chemical properties, which are crucial for understanding their environmental behaviour. Furthermore, the full range of chemicals released from tire pollution is still unknown, adding complexity to environmental impact assessments. This project seeks to address these research gaps by first estimating the missing physico-chemical properties of TDCs. To do so, a list of >200 compounds known to be used in synthetic rubber has been extracted from the PubChem database. To enhance the scope of this work, we conducted non-target analysis (NTA) on tire-wear particle (TWP) leachate extracts to identify additional TDCs, thus broadening our dataset for more comprehensive property prediction and fate modelling. NTA was conducted on both non-polar and polar TWP extracts using two-dimensional gas chromatography-mass spectrometry (GCxGC-ToF-MS) as well as liquid chromatography-high resolution mass spectrometry (Orbitrap LC-HRMS). To estimate the physico-chemical properties for each chemical, this project leveraged prediction software tools such as the Estimation Programs Interface (EPI) Suite and the OPEn structure–activity/property Relationship App (OPERA). The partitioning tendencies of the TDCs were evaluated through interpretive chemical space plots. Environmental effect metrics, such as the fish bioconcentration factor and the acute oral systemic toxicity in rats were also predicted. Subsequently, this work applied level III steady-state fugacity models as environmental fate assessment tools to better understand the distribution, transformation, and persistence of these contaminants in different environmental matrices. This work will allow for the prioritization of these compounds in future environmental monitoring campaigns and empirical toxicity assessments as well as guide the refining of their chemical management strategies.

COMPUTATIONAL CHEMISTRY

From Organic Principles to Predictive Models: Advancing pKa and Geometry Calculations with Graph Neural Networks

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The discovery of new therapeutics is a lengthy and complex process, often requiring substantial experimental effort. To accelerate this process, *in silico* methods like virtual screening and molecular docking have enabled chemists to evaluate potential bioactive compounds in a fraction of the time. However, these methods face a trade-off between accuracy and computational efficiency. Our research focuses on developing models that are both fast and precise, particularly for predicting small molecules' key properties, such as optimized geometries and pKa values, which significantly improve the reliability of computational predictions.

To address this challenge, we incorporate established organic chemistry principles—such as hyperconjugation, electronegativity, and the chemical environment—into our predictive models. These fundamental organic chemistry principles enhance model accuracy by enabling a more nuanced understanding of molecular behaviour. In this work, we present how modelling the chemical environment with molecular graph structures enables the use of Graph Neural Networks (GNNs) to predict essential chemical properties. This architecture allows us to accurately compute conformational energy barriers and pKa values directly from molecular structures, providing a robust framework for computer-aided drug and catalyst design.

NANOCHEMISTRY

Phytoglycogen nanoparticles: a promising nanocarrier for the inhalation delivery of antibiotics

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Lower respiratory bacterial infections have drawn a lot of attention due to their severe complications and the ongoing emergence of resistance to antibiotics. New strategies of antibiotic delivery are being explored to combat these infections especially through inhalation, which could provide a high localized effect with minimal systemic toxicity. Amikacin (AMK), an aminoglycoside antibiotic, exhibits an outstanding antibacterial activity; however, its use is limited due to low bioavailability and high toxicity. We report the use of the biodegradable, non-toxic, generally regarded as safe phytoglycogen nanoparticles for the inhalation delivery of AMK. Electrostatic association was employed for the loading of AMK into the carboxymethyl phytoglycogen with different mass ratios. Nanoformulations were evaluated for their colloidal stability, loading capacity, and release characteristics as well as their antibacterial activity and cytotoxicity.
The nanoformulation showed a very high loading capacity and hydrodynamic diameter of 60 nm with a low polydispersity that are independent of the preparation parameters. Additionally, the selected nanoformulation not only maintains the AMK antibacterial but also confers a biphasic release of AMK from the nanoparticles, an essential property for antimicrobial activity. These data support phytoglycogen nanoparticles as excellent candidates for the inhalation delivery of antibiotics to treat various bacterial lung infections.

Fluorescent carbon dots: A novel bioimaging tool to reveal the mechanism of action of anticancer drugs in cells

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The mechanisms of many cancer drugs at the subcellular level are still unclear, which is vital for enhancing their efficacy and selectivity. We are developing a novel method to visualize drug interactions using carbon dots (CDs), carbon-based nanoparticles known for their excellent optical properties and low cytotoxicity, making them ideal for bioimaging. Our research shows that amine-passivated CDs with negative surface charges accumulate in the cytosol of human cells and emit blue fluorescence with high quantum yields. Their surface can be functionalized to link with a drug of interest. In this research we are covalently linking these CDs to Doxorubicin (Dox), an established anticancer drug, to monitor their conjugation, cellular uptake, and localization. Additionally, we have designed thienoisoquinoline compounds that selectively target triple- negative breast cancer cells, disrupting microtubule polymerization and inducing unique mitotic arrest. This approach will help determine whether these compounds target centrosomes or microtubules across different cell types, providing insights into the mechanisms of anticancer drugs to advance structure-activity- relationship studies for improved drug development.

Characterizing the cellular interaction of DNA nanostructures from in-vitro to in-vivo

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McGill University

DNA nanostructures are an excellent system to carry and deliver nucleic acid therapeutics *in vivo* owing to their innate biocompatibility, stimuli responsiveness, and the ability to precisely control their physical properties (size, shape, surface ligands, etc.)There is a need to systematically study these nanostructures *in vivo* to obtain precise structure-activity relationships (SARs). However, present methods for studying SARs are tedious and time consuming. Here, we will describe a method known as ‘DNA barcoding’ and show that using this method we can identify differences in uptake of DNA nanostructures in different conditions including different transfection conditions and concentrations. Even though uptake is an important aspect of delivery, another aspect of it is endosomal escape. Therefore, as a next step, we will describe a method where we will utilize a “chloroalkane penetration assay” (CAPA) to study endosomal escape. At the end, we also studied the biodistribution and functional uptake of these structures *in-vivo*, allowing us to get a clearer picture of the structure-activity relationship.Thus, with the ability for high-throughput screening of barcoded structures and a strategy to measure their endosomal escape we aim to rapidly arrive at DNA nanostructures that selectively deliver nucleic acid therapeutics to the disease site.

Development of optical biosensor based on GQD/ZnO for potential detection of *Salmonella typhi*

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In this work, graphene quantum dots and zinc oxide were synthesized for the potential detection of *Salmonella typhi*, UV-Vis results were an absorption band at 219 nm correspond to the transitions of the π-π* of the C=C bond of graphene was observed, PL was used to know the fluorescence and the wavelength of maximum excitation and to know the appropriate conditions for the detection of *S. typhi* obtaining an interval between 313 to 317 nm for different synthesis conditions, TEM shows the morphology and particle size of the ZnO and GQD and the nanocomposite between this two materials, the ZnO have some cavities with a similar size to the QD favoring the formation of the nanocomposite.

Gold-Supported Lipid Membranes Formed by Redox-Triggered Fusion: A Study of The Thermotropic Properties

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L'utilisation de models de bicouches lipidiques supportées (SLBs) sur un substrat permet une meilleure approche d'étude vis-à-vis ces systèmes complexes. Plusieurs intérêts découlent de l'utilisation des
SLBs, notamment pour des applications biotechnologiques ou des investigations biophysiques. L'utilisation de différents substrats, ayant conséquemment des propriétés physicochimiques différentes, a un impact sur les propriétés thermotropiques des SLBs. Le projet consiste à étudier les propriétés thermotropiques de membranes lipidiques supportées par une monocouche auto-assemblée (SAMs) de ferrocénylalcanethiolates sur un substrat d'or. Une bicouche de DMPS a été induite par la suite d'une fusion de vésicules unilamellaires (SUVs, 50 nm) déclenchée par un processus redox. L'AFM à température-contrôlée a été utilisée
pour déterminer un changement de la morphologie suivant l'accroissement de la température ; la littérature prévoit une dépression (1nm) graduelle lors de la transition de température. Il a été démontré dans la littérature qu'ils existent deux points de transition : premier feuillet (externe), puis second feuillet (interne), ce dernier fixé au substrat. Les résultats préliminaires concernant l'utilisation d'un substrat d'or recouvert d'une SAM au détriment du mica n'indique pas un point de transition concluant.

Layer-by-Layer-modified lipid nanoparticles for miR-181a delivery in glioblastoma treatment

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Introduction: Glioblastoma multiforme (GBM) is the most common and lethal primary brain cancer. Current pharmacological interventions marginally increase the 12-month overall survival of patients with GBM. Among the novel therapeutic strategies being pursued, micro-RNAs, a class of non-coding RNAs, are receiving considerable attention for their regulation of several pathways implicated in tumorigenesis and survival. Notably, microRNA-181a-5p (miR-181a) has consistently been reported to be downregulated in GBM clinical samples, and its overexpression negatively affects tumor growth both in vitro and in vivo.
Objective: To improve the delivery of miR-181a to GBM cells, we sought to develop a modified lipid-based nanocarrier capable of encapsulating and delivering miR-181a to GBM cells in vitro and in vivo.
Methodology: Hyauronan-decorated lipid nanoparticles (HA-LNPs) were constructed by covering ionizable LNPs with different polyelectrolytes using the layer-by-layer technique. HA-LNPs were characterized by DLS, encapsulation efficiency, and AFM. The gene transfection efficiency of HA-LNPs was validated *in*
vitro and the effect of miR181-loaded HA-LNPs was evaluated *in vivo.*
Results: HA-LNPs targeted GBM cells more efficiently than non-modified LNPs, mediating potent gene transfection *in vitro* and *in vivo*. Finally, delivery of miR-181a by HA-LNPs delayed tumor growth in the in vivo GBM subcutaneous tumor model.

The formation of nanodendritic silver structures from a silver salt solution via continuous-wave laser irradiation

M. Paziresh
Queen's University

The synthesis of metal nanoparticles is a key research area due to their exceptional optical, electronic, magnetic, and catalytic properties, closely linked to their size and morphology. Silver nanoparticles (Ag NPs) are particularly significant because of their wide applications in optoelectronics, energy harvesting, catalysis, chemical and biological sensing, imaging, and biomedicine. Their superior electrical and thermal conductivity, along with their ability to enhance surface-enhanced Raman scattering (SERS), makes them crucial for sensitive chemical analyses and molecular detection.

Silver dendrites, with their complex hierarchical structures, offer unique benefits. These dendrites, characterized by sharp tips and closely spaced branches, create numerous hot spots and exhibit significant curvature, leading to outstanding plasmonic properties and a high surface area. These features are particularly advantageous for catalytic and photocatalytic applications Conventional methods for synthesizing these structures include chemical reduction, surface deposition, auxiliary techniques such as magnetic and ultrasonic fields, and the use of pulsed and continuous laser irradiation

In this study, we aim to achieve the targeted growth of silver dendritic structures using low-intensity continuous blue laser irradiation. This approach provides precise control over synthesis parameters, addresses challenges related to uniformity and stability, and opens new avenues for advanced applications in nanotechnology.

Towards BioFoundry on a Chip – A Digital Microfluidic Platform for DNA Synthesis by Phosphoramidite Chemistry

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Deoxyribonucleic acid (DNA) is a natural polymer with a wide range of applications from cell transformation to therapeutics and biosensors. DNA can be chemically synthesized through phosphoramidite chemistry, in which the first unit attached to a solid support and extended one unit at a time by means of a four-step reaction cycle.

In biology, due to high system complexities, many workflows adopt an iterative trial-and-error approach. Much effort has been put into developing solutions to automate each step in this laborious process, leading to the establishment of Biofoundries. Nevertheless, these infrastructures may not always be accessible to all and some processes, such as the de novo synthesis of DNA, are still often outsourced.

The field of microfluidics in part aims to alleviate some of these issues through automation, miniaturization and integration of traditional laboratory workflows. This project proposes a digital microfluidic (DMF) platform capable of small scale de novo DNA synthesis by phosphoramidite chemistry with micro-volume liquid handling through the application of an electric potential over dielectric. Controlled pore glass beads have been magnetized and functionalized with deoxythymidine. Preliminary synthesis results have demonstrated the compatibility of the phosphoramidite reagents with the DMF system and a 5-mer has been synthesized.

POLYMER CHEMISTRY

Photo initiator and Acrylate Free Photo-cross linkable Hydrogel

U. Mody*, M. Wolf
The University of British Columbia

A novel photo crosslinking hydrogel system that eliminates the need for photo-initiators and acrylates is synthesized using Alginic Acid. Conventional hydrogels often rely on photo-initiators and acrylate-based crosslinkers to harness ultraviolet light energy to polymerize monomers. Most commercial applications use acrylate for polymerization of monomers however monomers of acylate may pose toxicity, limited biocompatibility, and potential for adverse reactions.

To address these issues, we propose the replacement of acrylate with D/L alpha lipoic acid as the crosslinking agent in biodegradable polymers. Alpha Lipoic Acid absorbs UV light to undergo ring-open polymerization of sulfur-sulfur bonds. Alginic Acid is chosen as the base polymer to evaluate the effectiveness of the alpha lipoic acid in photocrosslinking conditions.

The structure of the polymer is evaluated using NMR, FTIR, and UV Vis absorbance Bands. Polymers are photo-crosslinked into dog bone-shaped structures and evaluated using stress/strain curves (mechanical properties), swelling behavior, and biocompatibility.

The results demonstrate an innovative approach to circumvent the limitations associated with conventional hydrogels and enhance safety for biomedical and tissue engineering applications. This advancement holds significant promise for developing safer, more versatile hydrogels with broad applications in regenerative medicine.

Scaling Carboxylated Cellulose Nanocrystals to Make Functional Microspheres

M. Wolff*, M. Andrews
McGill University

Functional materials developed from renewable resources are crucial to circular economies as they embrace sustainable practices for human and planetary well-being. The most abundant of renewable bio-derived polymers, cellulose, has enormous potential to support many of the UN sustainability goals. The Andrews group has scaled a sustainable manufacturing process to produce free-flowing powders of carboxylated cellulose nanocrystals (cCNC) by catalyst-free dilute aqueous hydrogen peroxide hydrolysis and oxidation of cellulose fibres. We use spray-drying to provide aerosol-assisted quenching of cCNC into persistent non- equilibrium states. This allows one to kinetically trap and co-locate different types of matter in a cCNC microsphere to confer new properties on the nanocomposite structure. A diverse selection of cCNC microspheres with a range of properties can be achieved through modifying the composition of the disperse state feed solution. Pigment microparticles are made by spray-drying cationic polyelectrolyte complexes of cCNC with anionic dye molecules. Spray-drying a suspension of cCNC, poly(acrylic acid) (PAA), and poly(hexamethylene biguanide) hydrochloride (PHMB) allows us to combine the biocidal effects of PHMB with the pH responsive effects of PAA. The influence of PAA polymer molecular weight on the stability of PHMB-PAA cCNC suspensions is studied using dynamic light scattering, zeta potential, and turbidimetry measurements.

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Przybylski's Star shouldn't exist.

Meet HD 101065, better known as Przybylski's Star, a cosmic puzzle that has left astronomers and chemists scratching their heads since its discovery in 1961. This seemingly ordinary A-type star, located about 355 light-years away, harbors interesting elements revealed by spectroscopy.

Element	Half-Life
Plutonium (Pu)	≤ 80 million years
Neptunium (Np)	≤ 2.1 million years
Americium (Am)	≤ 7,370 years
Actinium (Ac)	≤ 21.7 years
Einsteinium (Es)	≤ 471 days

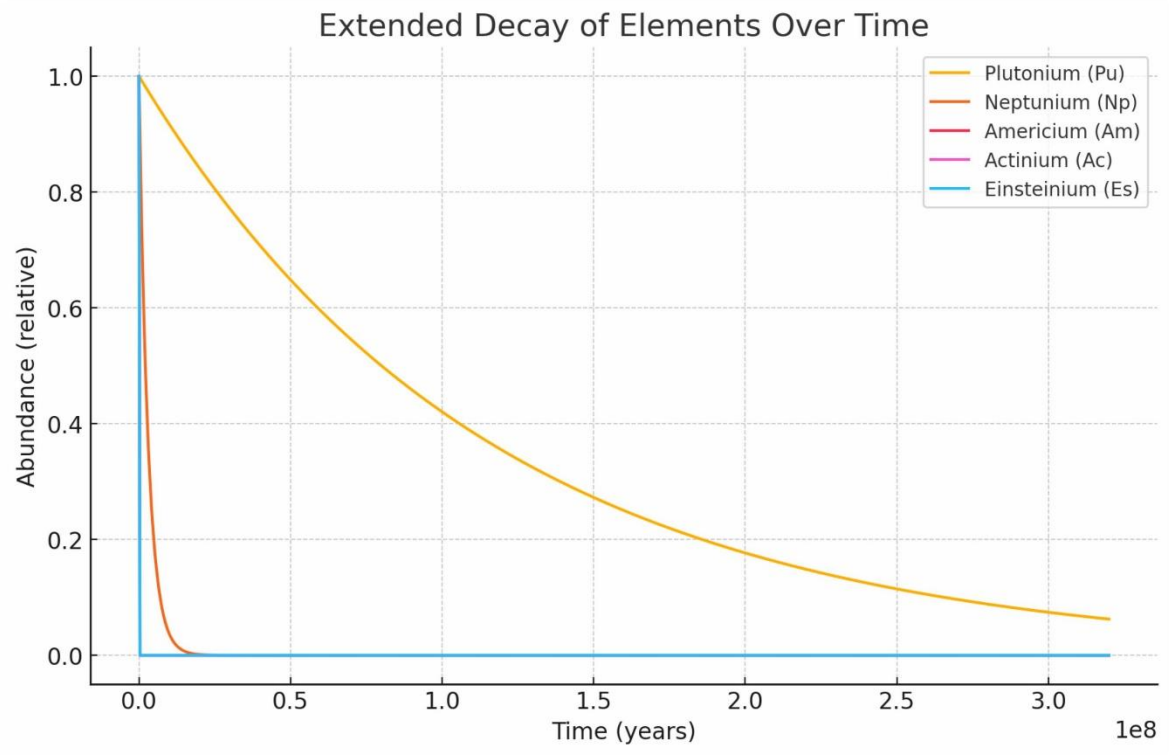
The strange part? These elements (and some others detected) are considered manmade—they shouldn't be found in nature.

The Impossible Elements

The half-life equation is how scientists model decay:

$$N(t) = N_0 \left(\frac{1}{2}\right)^{\frac{t}{t_{1/2}}}$$

It states that after every specific interval—known as the half-life—half of the original quantity of a substance remains. The following plot shows how the abundance of each of the above elements decreases over time, halving at each interval.



The universe is about 13.8 billion years old. Any traces of radioactive elements should have long decayed by now. Yet, spectral analysis shows an abundance of these short-lived elements, as if something—or someone—is continuously replenishing them.

Why This Matters

The presence of these elements challenges our understanding of:

- Stellar nucleosynthesis
- Element stability in extreme conditions
- Potential extraterrestrial technological signatures

How are these elements still present in a star billions of years old? Some scientists propose this could be evidence of an advanced civilization using the star as a "waste bin" for radioactive elements. Others suggest unknown nuclear processes at work. What do you think?

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We would like to extend our heartfelt thanks to all participants, judges, sponsors, speakers, panelists, and attendees for making this year's conference a resounding success. Our sincere gratitude goes to the departments, organizations, and institutions whose support and expertise helped bring this event to life. A special thanks to our dedicated volunteers and organizing committee for their hard work and commitment. We hope you had a wonderful experience at this year's event and look forward to welcoming you back for the 27th CBGRC!

The Organizing Committee

Nous tenons à remercier sincèrement tous les participants, juges, sponsors, conférenciers, panélistes et participants pour avoir fait de la conférence de cette année un succès retentissant. Notre profonde gratitude va aux départements, organisations et institutions dont le soutien et l'expertise ont permis de donner vie à cet événement. Un merci tout particulier aux bénévoles et au comité organisateur pour leur dévouement et leur travail acharné.

Nous espérons que vous avez vécu une expérience enrichissante lors de l'événement de cette année et nous nous réjouissons de vous accueillir à nouveau pour la 27e édition du CBGRC.

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