UNIVERSITÉ Concordia UNIVERSITY

CBGRC
Chemistry and Biochemistry Graduate Research Conference

November 21st, 2025

27th ANNUAL CBGRC

CHEMISTRY AND BIOCHEMISTRY GRADUATE RESEARCH CONFERENCE



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DR. LEE FADER

VICE PRESIDENT OF CHEMISTRY AT CONGRUENCE THERAPEUTICS - BIOTECH COMPANY FOCUSED ON AI-DRIVEN DRUG DISCOVERY, PROTEIN STRUCTURE MODELING, AND RARE DISEASE THERAPEUTICS

DR. NICOLAS MOITESSIER

PROFESSOR AT MCGILL UNIVERSITY, CO-FOUNDER AND CSO AT MOLECULAR FORECASTER SPECIALIZING IN STRUCTURE-BASED DRUG DESIGN, DOCKING TECHNOLOGIES AND COMPUTATIONAL CHEMISTRY INNOVATION



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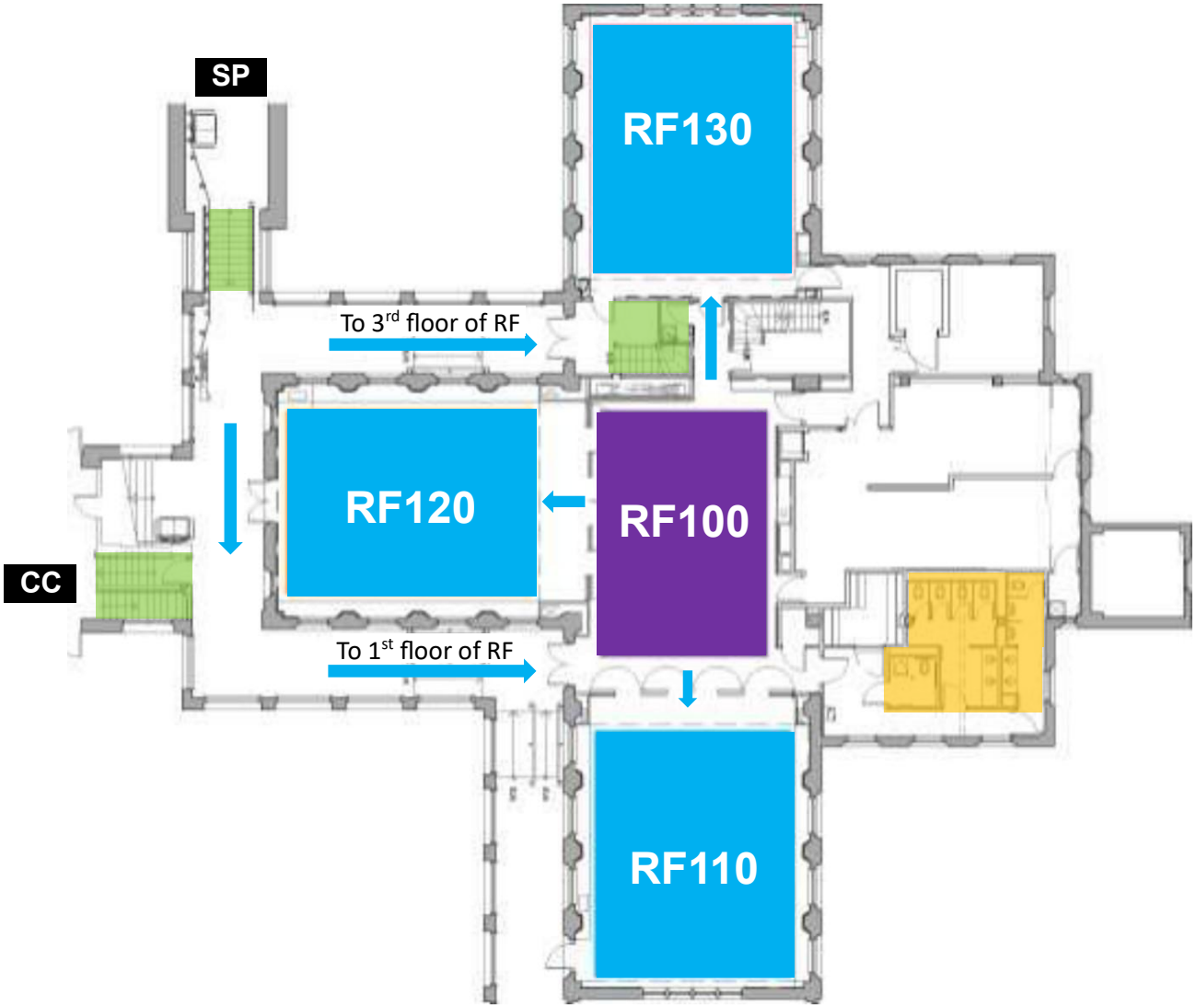
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Campus Maps

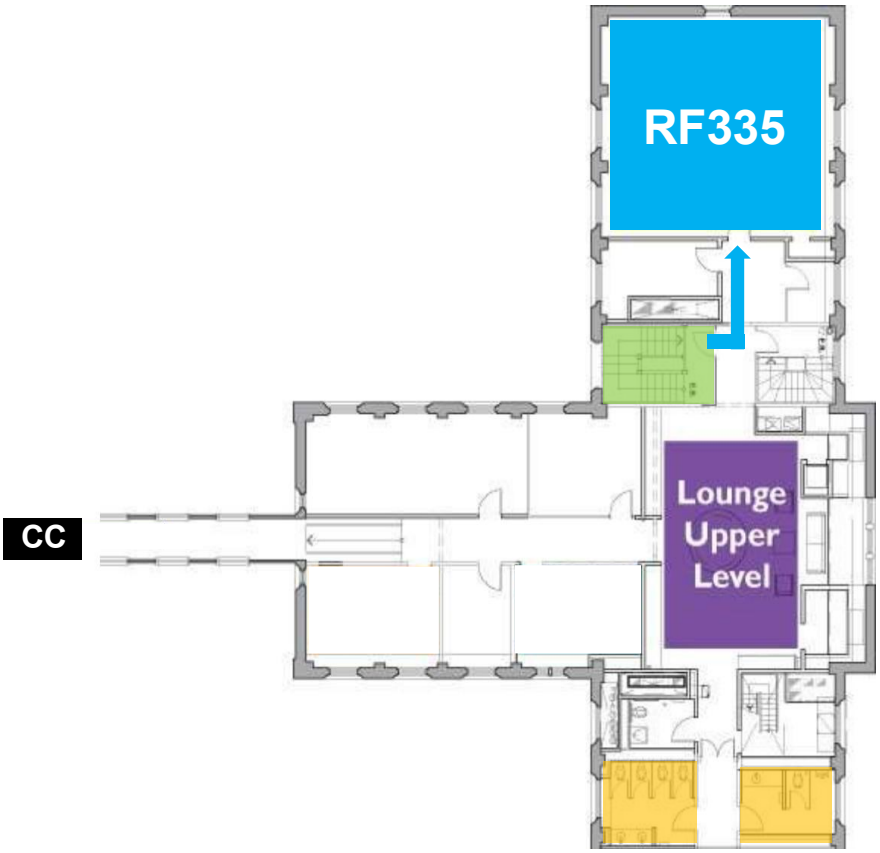

P2 -Jesuit Lot
Daily Parking
HC
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Registration
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Coffee Table
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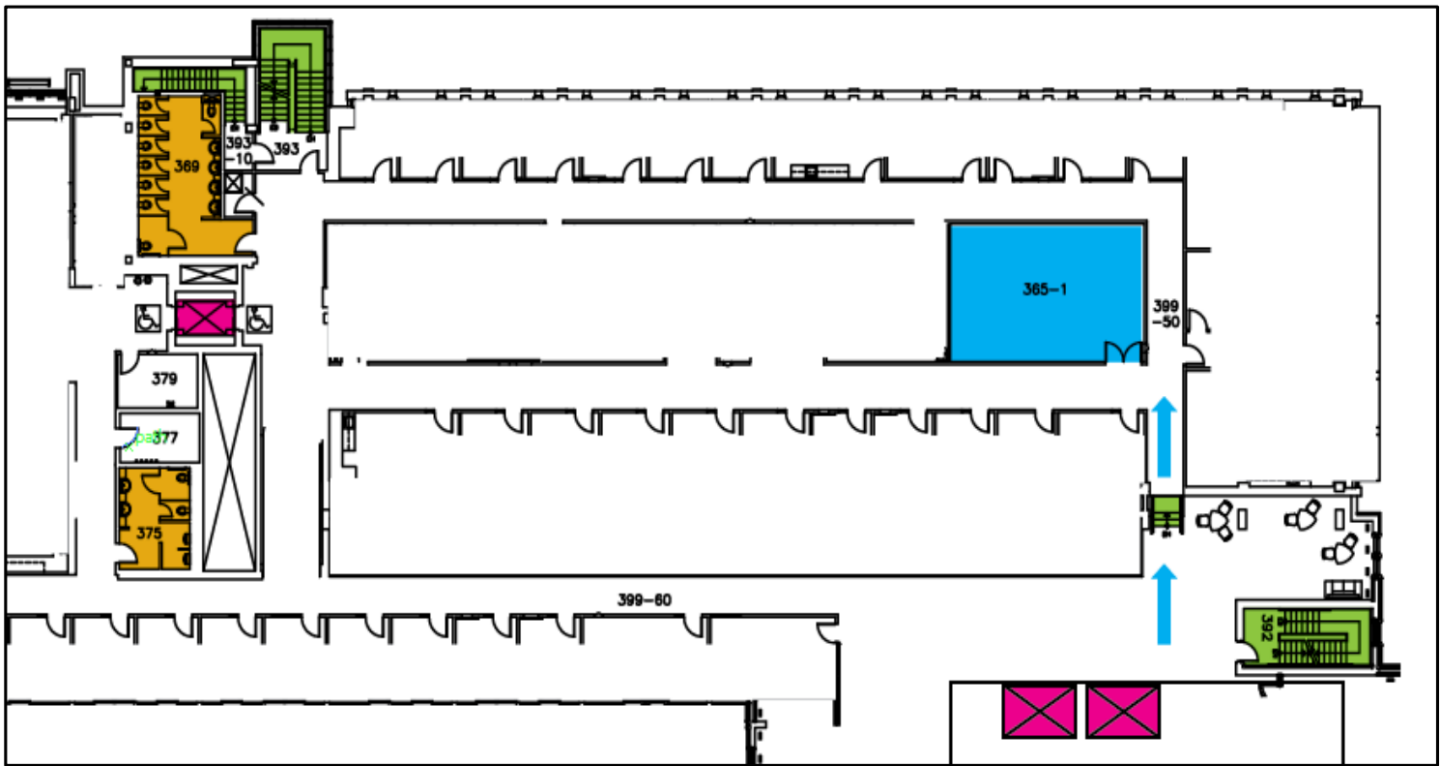
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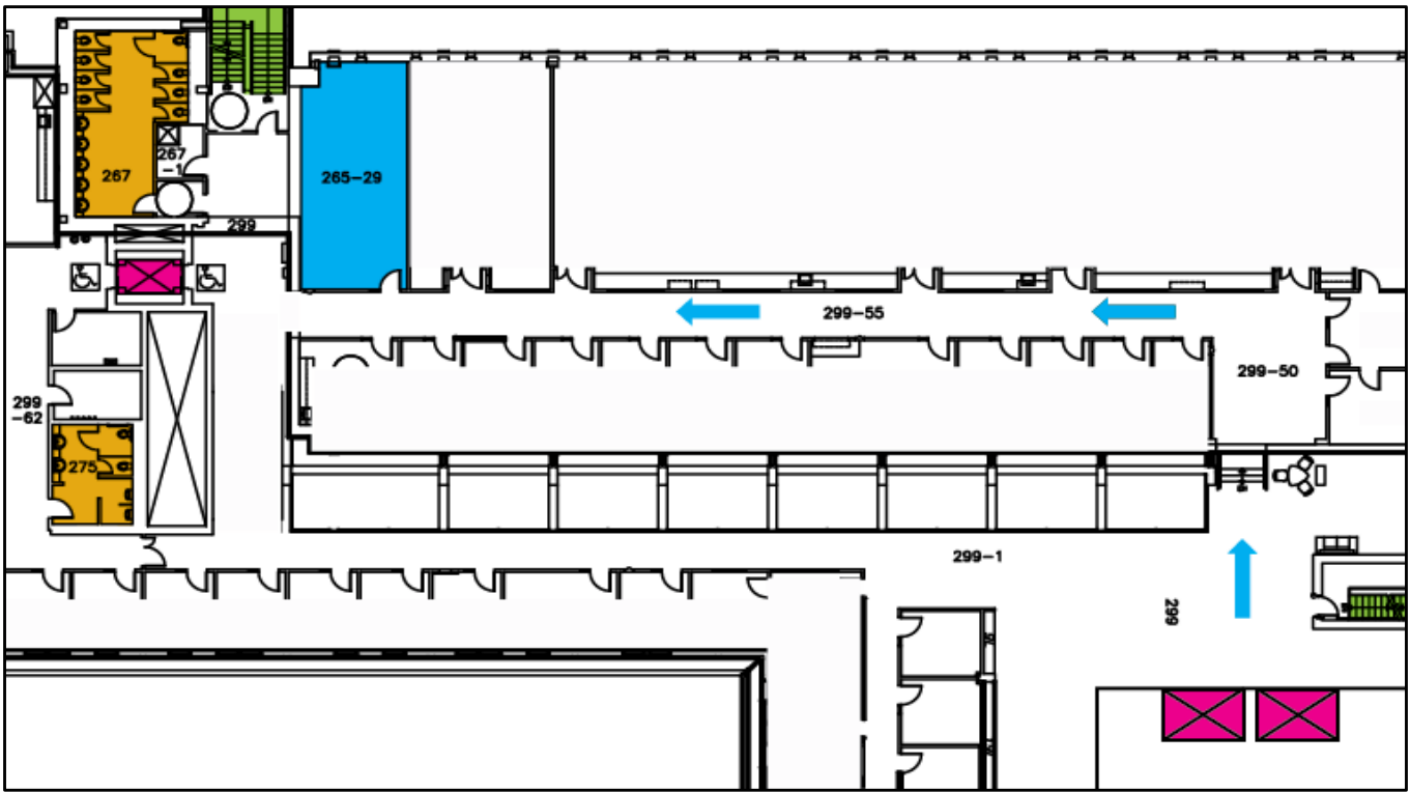
RF Conference Center – 3rd Floor



SP 365.01



SP 265.29



Welcome Note

Dear friends and colleagues,

We are glad to welcome you to the 27th Annual Chemistry and Biochemistry Graduate Research Conference (CBGRC)! 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 27e Conférence annuelle sur la recherche des cycles supérieurs en chimie et biochimie (CBGRC)! 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

Keynote Speakers

Dr Nicolas Moitessier



Professor at McGill University

Co-Founder and CSO at Molecular Forecaster

Biography

Dr. Nicolas Moitessier received his Ph.D (1998) from Université Henri Poincaré-Nancy I (France) before moving to Montreal for post-doctoral studies at University of Montreal in medicinal chemistry, and asymmetric synthesis. In 2001, he moved back to Nancy to start an academic career (Chargé de Recherche, CNRS) then back to Montréal in 2003 to join the McGill Chemistry department. Moitessier's research interest in drug discovery includes computational methods development and medicinal chemistry focusing on the development of small molecules targeting RNA and inhibitors of an enzyme involved in Parkinson's disease. In 2010, Moitessier co-founded Molecular Forecaster, a McGill spin-off company distributing the software developed in his lab and providing research support to the pharmaceutical industry. Since 2016, he has been an Associate editor of the European Journal of Medicinal Chemistry. Over the years, he received several awards, including the Fessenden Professorship and the 2023 CIC Biological and Medicinal Chemistry Lectureship Award.

Abstract: Can we teach chemistry to computers?

Computational methods including machine learning (ML) models are gaining momentum in chemistry for the prediction of various molecular properties. However, while machines are learning, who is teaching? Aiming to revisit the way computational method development is practiced in chemistry, our strategy involves imparting chemistry knowledge to algorithms rather than leaving the machines learning unsupervised. We posit that teaching fundamental principles to machines to predict properties, analogous to the way we teach students, will provide more accurate methods. We will present this concept in the context of asymmetric synthesis. Algorithms will learn principles to search for lowest-in-energy conformations, compute potential energies, molecular properties and more.

Dr Lee Fader

Vice President of Chemistry at Congruence Therapeutics



Biography

Dr. Lee Fader brings nearly two decades of experience in the pharmaceutical industry, with a strong track record in drug discovery and development. Since May 2021, Dr. Fader has served as Vice President of Chemistry at Congruence Therapeutics, where they lead innovative programs in medicinal chemistry. Prior to this role, Dr. Fader held senior positions at Ventus Therapeutics and Inception Sciences, driving early-stage research and discovery efforts. Earlier in their career, Dr. Fader contributed significantly to Vertex Pharmaceuticals as a Research Fellow and spent over a decade at Boehringer Ingelheim, advancing from Research Scientist to Principal Scientist.

Abstract: Discovery of potent, orally bioavailable correctors of MC4R misfolding for the treatment of MC4R-deficient obesity.

The melanocortin-4-receptor gene (MC4R) is a key regulator of energy homeostasis, feeding behavior, and metabolism. Autosomal dominant mutations in the MC4R gene are the leading cause of severe childhood-onset obesity, characterized by rapid weight gain and persistent food-seeking behavior. To date, more than 170 distinct mutations have been identified from patient cohorts, the majority leading to improper protein folding and resulting in impaired trafficking to the plasma membrane. Ligand-induced correction of this defect could reverse the obesity phenotype in impacted patients. At Congruence Therapeutics, we use Revenir™, our in silico drug discovery engine to discover small molecule MC4R correctors which escort misfolded proteins to their correct locus to restore their function. The discovery and optimization of a series of correctors of MC4R misfolding will be described.

Schedule Overview

Time	Room	Event
8:00 - 18:00	SP Atrium	Registration
9:00 - 10:30	See presentation schedule	Student Presentations - Session A
10:30 - 11:00	SP Atrium	Coffee Break and Sponsors Exhibition
11:00 - 12:00	HC 157	Keynote Speaker: Dr. Nicolas Moitessier
12:00 - 13:00	RF and SP Atrium	Lunch and Sponsors Exhibition
13:00 - 14:15	See presentation schedule	Student Presentations - Session B
14:15 - 14:30	SP Atrium	Coffee Break and Sponsors Exhibition
14:30 - 15:30	HC 157	Keynote Speaker: Dr. Lee Fader
15:30 - 15:45	SP Atrium	Coffee Break and Sponsors Exhibition
15:45 - 17:30	See presentation schedule	Student Presentations - Session C
15:45 - 16:15	SP 365.01	Empowering Women in Organic Chemistry (EWOC) Information Session
17:30 - 19:30	RF 120	Poster Presentations
18:00 - 22:00	RF Conference Center	Wine and Cheese
20:00	RF Conference Center	Award Announcements

Schedule

Student Presentations

Session A | 9:10-10:30 am

Organic Chemistry — SP 365.01

9:10 E. Cordova Mosquera (*McGill University*): Expanding the Toolbox of Chemical Modifications for Nucleic Acid Therapeutics: Synthesis and Studies on 4′-Cα-Methoxy Nucleosides

9:25 D. Patel (*Brock University*): Synthesis and Mechanistic Insights into the Formation of 1,2-Bisphenylhydrazones

9:40 P. Saha (*University of Ottawa*): Cross-couplings of transiently stable organolithium compounds

9:55 E. Chen (*McGill University*): Palladium-Catalyzed Tsuji-Trost-Type Vinyl Epoxide Cross-Coupling with Umpolung Hydrazones

10:10 L. Ganeo Neto (São Paulo State University (UNESP)): Chirality in motion: lipase-catalyzed dynamic covalent kinetic resolution of 5-hydroxy-2(5*H*)-furanone

Chemistry Education — RF 110

9:55 S. Al Akkad (*University of Ottawa*): Transforming Chemistry Education through Interdisciplinary Training: Pathways for Future Scientists

10:10 L. Temple-Murray (*University of Ottawa*): The impact of using generative artificial intelligence on critical thinking and scientific reasoning in organic chemistry education

Biochemistry RF 130

9:25 H. Nizal (*McGill University*): How Many Cytosines Must Be Protonated? Site-Specific Insights into i-Motif Folding from NMR and UV-Vis Studies

9:40 T. Rutherford (*Concordia University*): Synthesis and Characterization of DNA Tetrahedra Containing O6-Alkylene 2′-Deoxyguanosine Cross-Links for Controlled Disassembly by a DNA Repair Protein

9:55 S. Dao-Tse (*Concordia University*): Synthesis and Characterization of C5-Modified Arabinonucleic Acids

10:10 K. Gremi (*McGill University*): RNA Aptamer-based Biosensing in Living Cells and Animals

Inorganic Chemistry RF 335

9:10 C. Copeman (*Concordia University*): Adsorptive Removal of Oxyanions from Water using a Zr-based Metal–Organic Framework

9:25 I. Oubaha (*Université de Montréal*): Highly efficient and photostable Ruthenium terpyridine complexes as photosensitizers for artificial photosynthesis

9:40 Á. Lozano-Roche (*Universitat Autónoma de Barcelona, Université de Montréal*): Size and Ligand Effects on Ru Nanoparticles for Hydrogen Evolution

9:55 C. Vieira Diniz (*Concordia University*): Thiol-Functionalized Metal–Organic Frameworks as Drug Delivery Platforms for Ophthalmic Therapeutics

10:10 Saha (*Université de Montréal*): A bright exception: Spectroscopic rational of anti-Kasha photophysics of Co(III)-Amidine-N-Oxide complexes

Molecular Biology SP 265.29

9:10 M. Simoes (*Concordia University*): Transcriptomic Profiling of the Plasmid Induced Cellular Burden and the Impact on Natural Product Production

9:25 K. G. Antenor (*Toronto Metropolitan University*): Vacuolar pH regulates clathrin-mediated endocytosis through TORC1 signaling during replicative aging

9:40 A. Naaz (*Concordia University*): Investigating the Role of Tango2 Protein in Yeast: A Model for Rare Metabolic Disease

9:55 D. Joseph (*Dartmouth Geisel School of Medicine*): A Deep Learning Approach to Identify Ganciclovir Incorporation in DNA and Understand Determinants of Cytomegalovirus Resistance

10:10 R. Carter (*Carleton University*): Spatiotemporal silencing of mRNAs during hibernation: Roles of stress granules and P-bodies

Organic Chemistry — SP 365.01

1:00 C. Rocq (*Université du Québec à Montréal*): Enantioselective Organocatalytic Synthesis of a [6-5-3] Tricyclic System via a One-Pot Tandem Sequence

1:15 A. Paquin (*Université du Québec à Montréal*): Hit Triage Method enables Discovery and Validation of DNMT3a Inhibitors

1:30 B. D'Onofrio (*Université de Montréal*): Structure/Activity Relationships in TPDYs for Strain-Promoted Cycloadditions

1:45 C. Nguyen (*Concordia University*): Development of Stimuli-Responsive Linkers for the Synthesis of Oligonucleotide Conjugates

2:00 N. Beaucage (*Université de Montréal*): Development of Copper-Based Complexes for Absorbing Red Light for Photocatalysis

Environmental Chemistry — RF 110

1:00 Y. Mirzaei (*Geotop Research Center and Concordia University*): Biogeochemical Characterization and Source Prediction of Organic Matter in a Land to Ocean Sediment Transect by Multivariate Analyses and Machine Learning

1:15 D. R. B. Doussiemo (*Université du Quebec à Montréal*): Influence of additives on the adsorption of contaminants by microplastics: role of surface properties

1:30 K. Hamzi (*UQAM*): Analysis of micro/nanoplastics using fluorescent probe

1:45 L. Cisneros (*Concordia university*): Biosurfactant Based Micellar-Enhanced Ultrafiltration (MEUF) for Metal Recovery from Alkaline Leachates

2:00 R. B. Opoku (*Concordia University*): Compilation and assessment of chemicals used in large quantities in Africa: Temporal trend-based prioritization and environmental risk characterization indicate urgent management and regulatory needs

Biochemistry RF 130

1:00 E. Ali (*Concordia University*): *Myxococcus*-Based Elicitation Enhances Antimicrobial Biosynthesis in *Aspergillus terreus*

1:15 M. Michichiuc (*University of Ottawa*): Toward In Vivo Olefin Metathesis: Targeted Catalyst Delivery via a Protein-Catalyst Conjugate

1:30 S. Hamroff (*McGill University*): Insights into liquid-to-solid transitions of ultra-short peptides coacervates yield a new class of peptides that enable next-generation solvent-free catalysis

1:45 M. Khammar (*Université de Sherbrooke*): Size Matters: Reconstructing a Functional Tripartite Multidrug Efflux Pump in a Lipid Bilayer

2:00 G. Hanna (*McGill University*): Unraveling Lanthipeptide Biosynthesis: High-Resolution Insights via Nuclear Magnetic Resonance

Computational/Analytical Chemistry RF 335

1:00 D. Boivin (*Concordia University*): Instrument Development for Targeted Heart-Cuts of Complex Samples from a Sheath-Flow-Interface Capillary Electrophoresis Array

1:15 L. Kuster (*Université du Québec à Montréal*): Theoretical investigation of *para*- and *ortho*-water reacting with C+ and CO+ ions in the interstellar medium

1:30 F. Alaghemand (*McGill University*): Computational Investigation of Reaction Mechanisms in Pd-, Ni-, and Au-Catalyzed Systems

1:45 S. Norouzi (Concordia University): Development and Evaluation of Machine Learning Models to Screen Environmental Risks of Chemical Features Based on Information Gained from Non-targeted Chromatography-Mass Spectrometry Analysis

2:00 T. Scherle (*University of Ottawa*): Machine Learning QSAR Modeling for Cannabinoids & the CB1/2Receptors

2:15 A. Radnoff (*University of Ottawa*): Determination of the pyrolysis products and decomposition mechanisms of per/polyfluorinated compounds using imaging photoelectron photoion coincidence spectroscopy (iPEPICO)

Nanochemistry/Polymer Chemistry SP 265.29

1:00 C. M. Santos Calado (*University of Ottawa*): Composition Control in Molecular Cluster-Aggregates: A Toolbox for Optical Output Tunability *via* Energy Transfer Pathways

1:15 N. Fischer (*Concordia University*): From Eggshell to Egg yolk: Spatially Programming the Distribution of Ruthenium Nanoparticles inside a Metal–Organic Framework via Direct Incipient Wetness Impregnation

1:30 T. Jacquemin (*UQAM*): Development of Organic-Inorganic PN Cage-Containing Polymers as Degradable Coatings

1:45 C. Garcia Henao (*Concordia University*): Tuning Trap Depth in Er^{3+}-Doped $NaLuF_4$ Nanoparticles through Codoping Strategies

Organic Chemistry — SP 365.01

3:45 - 4:15 Empowering Women in Organic Chemistry (EWOC) Information Session

Environmental/Physical Chemistry — RF 110

3:45 T. Delesa (*University of Quebec in Montreal*): Integrating Organic Waste Oxidation as a Pathway for Hydrogen Production from Wastewater

4:00 E. White Buenger (*University of Ottawa*): Improving The Understanding of Isoprene Pyrolysis Using Threshold Photoelectron Spectroscopy

4:15 S. Gondarry (*University of Ottawa*): Experimental Insights into the Fragmentation Mechanisms of Lignin-Derived Radical Cations: A Quantitative iPEPICO Study of 4-Ethylguaiacol and Eugenol

4:30 M. Creran (*Concordia University*): Novel Doping Agents for Degradation-Assisted Doping of Organic Semiconductors

Biochemistry — RF 130

3:45 S. Tikoo (*Concordia University*): Synthesis of Oligonucleotide Conjugates Containing Selenium Modified Linkers

4:00 J. F. Sanchez Tejeda (*McGill University*): Harnessing Lipid Peroxidation for Photoactivatable Ferroptotic Cell Death

4:15 A. Clairoux (*McGill University*): A capture-based approach for the separation of ligand-induced riboswitch conformations

4:30 P. Singh (*Concordia University*): Adaptive Evolution of *E. coli* Under Antibiotic Pressure Reveals Media Specific Patterns of Collateral Phenotypes

4:45 A. Woodhead (*Concordia University*): Novel Antimicrobials from Arctic Bacteria *Alteromondales*

Inorganic Chemistry RF 335

3:45 C. Pomilio (*Concordia University*): Iron Coordination Complexes as Aqueous Electrolytes for Redox Flow Battery Applications

4:00 V. Urunikulavan (*University of Ottawa*): Synthesis and study of single molecule magnetic behaviour in lanthanide metallocene complexes with 3,6-bis(3-pyridyl)tetrazine radical

4:15 N. Bajaj (*University of Ottawa*): Hard single-molecule magnet behavior and strong magnetic coupling in pyrazinyl radical-bridged lanthanide metallocenes

4:30 J. Ortega-Ramirez (*University of Ottawa*): A Systematic Study on the Molecular Symmetry and Magneto-Optical Behavior of Lanthanide(III) Complexes: Implications for Magnetic Circularly Polarized Luminescence

4:45 C. Brayner (*Université de Montréal*): Evaluating Structure/Activity Relationship of Heteroleptic Copper (I)-Based Complexes

Poster session | 5:30 - 7:30

Organic Chemistry — RF 120

O01 S. Alfonso (*University of Ottawa*): Silylation of alcohol-amines for the on-demand hydrogen generation: a simple and internally catalyzed reaction

O02 M. La Torre (*McGill University*): A new path towards meta-amino phenols

O03 V. Petkov (*McGill University*): Development of an Efficient Methodology for the Synthesis of Fully Deprotected Oligonucleotide Dimers and Trimers

O04 K. Prystupa (*University of Ottawa*): Streamlining Hydrogenation: Data-Driven Chemoselectivity Guide for Synthetic Chemists

O05 V. Wu (McGill University): Diaryl ether synthesis and functionalization from phenols and catechols via*ortho*-diazoquinones

Chemistry Education — RF 120

CE01 E. KM Delaire (*Institut National de Recherche Scientifique*): Assessing the Impact of Atropisomer Chirality on Drug Discovery and Development

Environmental Chemistry — RF 120

E01 A. Bisio (*UQAM*): Developpement of new membranes with enhanced ammonia permeability for separation by membrane distillation.

E02 A. Fowler-Clarke (*Concordia University*): Distinct Chemical Composition Profiles of Dust from Varied Sources Revealed through Targeted and Non-Targeted Analysis

E03 R. Paiva (*UFSC - Universidade Federal de Santa Catarina*): Toxicological effects of drugs of abuse on aquatic organisms: bioassays with Lemna minor and Daphnia magna

Biochemistry RF 120

B01 K. AMIENS (*INRS (Institut National de la Recherche Scientifique)*): Expanding Antiviral Strategies through NMR Fragment-Based Drug Discovery: The Case of SARS-CoV-2

B02 B. Albert (McGill University): Identifying and characterizing AML-binding aptamers for targeted delivery of RNA therapeutics

B03 N. Muñoz-Patiño (*McGill University*): Contrasting ion effects in moist-solids vs. conventional dilute aqueous conditions for enzymatic cellulose depolymerization

B04 R. N. Olegario (*McGill University*): Insights into mechanoenzymatic and mechanochemical depolymerization of polyhydroxybutyrate

B05 H.-W. Petit-Frere (*UQAM*): Evaluation of the importance of SUMO interaction motifs (SIMs) in the design of novel synthetic SUMO E3 ligases and identification of promising candidates for biotechnological applications

B06 V. Zhang (*McGill University*): The Role of Metal Ions in DNA-Guided Assembly of Carbonic Anhydrase II Active Site

Inorganic Chemistry RF 120

I01 M. Fiou (*Université Laval*): Effect of tetraphenylborate (BPh_4^-) on the catalytic and biological activity of organoruthenium complexes

I02 D. Girish (*Laval University*): Hydrosilane-mediated activation of B-O bonds for sustainable Boron recycling in cross-coupling reactions

I03 C. Gros (*Université de Montréal*): Innovative N,O-Bidentate Ligands for Enhancing the Photoactivity of First-Row Transition Metal Complexes

I04 C. McDonald (*Brandon University*): Development of carbene-supported half-sandwich Rh complexes for H2 storage applications

I05 E. Mohamad (*University of Ottawa*): Versatility of PN Ligands in Photocatalysis: Tailored Ni(II) and Ru Complexes for H2 Generation and CO2 Conversion

I06 I. Oubaha (*Université de Montréal*): Homoleptic cobalt(III) bisguanidylpyridine complexes for photocatalytic and photoredox processes

I07 J. Singh (*Concordia University*): Metal–Organic Frameworks for Direct Air Capture of Carbon Dioxide

I08 L. Thomas (*Concordia University*): Sustainable Production of a Zirconium Metal–Organic Framework Through Optimization of Washing Steps

Analytical Chemistry RF 120

A01 C. Leung (*Concordia University*): Feasibility of Protein Detection from a Single-Cell via Capillary Zone Electrophoresis Laser-Induced Fluorescence

Computational Chemistry RF 120

C01 J. Genzling (*McGill University*): Virtual Chemist: computer-aided design in asymmetric catalysis

C02 -A. Najera (*McGill University*): Advancing Aptamer Design Through Machine Learning Methods

C03 -M. E. Toloue Sadegh Azadi (*McGill University*): Predicting the folding of single-stranded DNA aptamers using a machine-learned coarse-grained force field

C04 -S. Zhang (*McGill University*): SO(3) Equivariant Embeddings for Transition State Prediction

Molecular Biology RF 120

M01 R. Carter (*Carleton University*): Identification of freeze-responsive microRNAs in vertebrate hearts: Novel insights into cardiovascular disease

M02 S. Diaconescu-Grabari (*McGill University*): Treating Infections by Inhibiting Growth Under Infection-Relevant Conditions

M03 D. Gokbayrak (*Concordia University*): Size-Based Flow Cytometry Sorting for Distinguishing Quiescent and Non-Quiescent Yeast Subpopulations

M04 G. Schick (*Concordia University*): Spatiotemporal regulation of Ect2, a proto-oncogene that is critical for cytokinesis

Polymer Science RF 120

PS01 L. (. Huang (*McGill University*): Spatiotemporally controlled formation of DOPA-based biomaterials

Abstracts – Oral Presentations

Organic Chemistry

Development of Copper-Based Complexes for Absorbing Red Light for Photocatalysis

N. Beaucage*, Z. Singh, J. Bourdon, S. K. Collins

Université de Montréal

Photocatalysis mediated by low energy light wavelengths has potential to enable safer, sustainable synthetic methods. Phenanthroline-derived ligands was used to construct homoleptic copper complexes. The complexes promotes energy transfer photocatalysis enabling oxidative dimerization of benzylic amines, sulfide oxidation, phosphine oxidation, boronic acid oxidation and atom-transfer radical addition under red light irradiation.

Palladium-Catalyzed Tsuji-Trost-Type Vinyl Epoxide Cross-Coupling with Umpolung Hydrazones

E. Chen*, C.-J. Li

McGill University

Selective functionalization of synthetically useful vinyl epoxides *via* carbon–carbon (C–C) bond formation has been a major challenge for many years due to their unique inherent chemical reactivity. Non-stabilized carbanions in the form of organometallic reagents have been shown to be robust and versatile reagents in C–C bond formation; however, they are employed in super stoichiometric quantities, require the protection of active functional groups, and generate copious amounts of metallic waste. Therefore, the development of mild carbanion sources as simple alternatives is highly desired. In this work, we report a highly chemo- and regioselective palladium-catalysed vinyl epoxide cross-coupling utilizing hydrazones as organometallic equivalents (HOME). Hydrazones, generated from carbonyl-containing renewable feedstocks, enable a more sustainable reaction, and provide an alternative to highly reactive and sensitive unstabilized organometallic reagents. A broad substrate scope, with high functional group tolerance, is demonstrated along with the late-stage functionalization of natural product derivatives.

Expanding the Toolbox of Chemical Modifications for Nucleic Acid Therapeutics: Synthesis and Studies on 4′-Cα-Methoxy Nucleosides

E. Cordova Mosquera*, A. Arora, M. Damha

McGill University

RNA–based drugs are revolutionizing medicine by directly correcting or silencing disease-causing genes at the transcriptomic level. More than 20 of these therapies are already approved, treating conditions once thought untreatable, such as spinal muscular atrophy, familial hypercholesterolemia, and hereditary angioedema. Despite their promising results *in vitro*, most oligonucleotide drugs still face significant challenges: they are unstable in the body, degrade rapidly, and sometimes fail to interact effectively with proteins required for therapeutic activity. Chemical RNA modifications are therefore essential for both elucidating the functional roles of RNA structure and ribonucleoprotein assemblies and improving RNA-based therapeutics. Current nucleotide analogues used for RNA stabilization often modify the 2′-hydroxyl group of the ribose, which is crucial for interactions with key proteins such as Cas9 in CRISPR-based gene editing. This trade-off limits the full potential of RNA therapeutics. We present a novel approach that targets the 4′ position of the ribose sugar—an underexplored site that can enhance RNA stability while preserving the crucial 2′-hydroxyl group. These

nucleoside analogues retain critical 2′-OH/Cas contacts. This project encompasses the chemical synthesis of 4′-O-methyl–modified nucleosides, their incorporation into RNA/DNA duplexes, and the evaluation of their effects on duplex stability, nuclease resistance, and CRISPR-Cas12a/Cas9 gene-editing efficiency.

Structure/Activity Relationships in TPDYs for Strain-Promoted Cycloadditions

B. D'Onofrio*, C. Cruché, H. Vanmollekot, S. Collins

Université de Montréal

Strain-promoted azide–alkyne cycloaddition (SPAAC) reactions are among the most powerful tools for bioorthogonal conjugation. Herein, we report the synthesis and structure–activity relationships of a family of terphenyl diyne (TPDY) macrocycles designed for strain-promoted cycloadditions. The electronic and steric factors on SPAAC reactivity were evaluated experimentally. In addition, an investigation of azide partners highlighted key steric and electronic parameters that govern diyne-based strain-promoted cycloadditions, providing design principles for next-generation bioorthogonal reagents.

Chirality in motion: lipase-catalyzed dynamic covalent kinetic resolution of 5-hydroxy-2(5*H*)-furanone

L. Ganeo Neto*, H. Milagre

São Paulo State University (UNESP)

Furanones, oxidation products derived from biomass-based furfural, represent key intermediates in the synthesis of bioactive compounds such as acetomycin and dysidiolide. Due to the equilibrium between their cyclic and open-chain forms, these molecules undergo racemization, enabling their use in dynamic covalent kinetic resolution (DCKR). This approach relies on a reversible process in which the covalent bond at the stereocenter is continuously broken and reformed. Lipases, known for their high chemo-, regio-, and enantioselectivity, as well as catalytic promiscuity, have been widely employed for the resolution of racemic mixtures. In this study, we investigated the lipase-catalyzed DCKR of 5-hydroxy-2(5*H*)-furanone. Enzyme screening revealed distinct selectivities: *Pseudomonas fluorescens* lipase preferentially catalyzed the (*R*)-enantiomer (conversion = 92%,89% *ee*), while *Candida rugosa lipase* selectively favored the (*S*)-enantiomer (conversion = 73%, 85 % *ee*).*Thermomyces lanuginosus* lipase exhibited high catalytic efficiency, achieving complete esterification within 2 hours. Additionally, various acyl donors were assessed to examine their influence on enantioselectivity. A clear inverse correlation was observed between acyl chain length and enantiomeric excess: longer chains resulted in decreased *ee* values. This study highlights the potential of enzymatic DCKR as a selective and efficient approach for the synthesis of enantiomerically enriched furanone derivatives.

Development of Stimuli-Responsive Linkers for the Synthesis of Oligonucleotide Conjugates

C. Nguyen*, C. J. Wilds

Concordia University

Oligonucleotide conjugates have demonstrated significant potential for drug delivery, biosensing, and gene therapy applications. These molecules consist of an oligonucleotide that is chemically linked to a targeting molecule, such as a peptide or polymer. A key element of oligonucleotide conjugates is the covalent connection by a linker which can be cleaved in response to a particular stimulus, crucial for ensuring efficient delivery and controlled release. Building on previous work that explored the disulfide group, we are investigating the application of selenium-based chemistry. Diselenide bonds offer faster reaction kinetics for cleavage relative to

disulfide, ideal for biomedical applications. A synthetic approach to prepare a diselenide linker starts from 1,6-hexanediol which undergoes a series of reactions including trityl protection, iodination and selenation to ultimately produce a phosphoramidite derivative of a versatile linker that can be incorporated into an oligonucleotide via solid-phase synthesis. Oligonucleotides containing this diselenide linker at the 5'-terminuswill be conjugated to small molecules and polymers, and selective cleavage of the linker under reducing conditions will be assessed by PAGE. This selenium modified linker will add to the toolkit of approaches for stimuli-responsive release of oligonucleotides conjugated to delivery platforms, potentially enhancing the efficacy and specificity of nucleic acid-based therapeutics.

Hit Triage Method enables Discovery and Validation of DNMT3a Inhibitors

A. Paquin[1]*, C. Jallet[2], S. Gallant[3], L.-J. Bourgeois[1], Y. E. A. Jimenez[1], J. Plamondon[1], F. Shahout[4], L. Cappadocia[1], S. Woo[3], M. Lussier[1], S. Laplante[4], P. B. Arimondo[2], A. Gagnon[1]

[1]Université du Québec à Montréal, [2]Institut Pasteur, [3]NMX Research and Solutions, [4]institut national de la recherche scientifique

Aberrant methylation patterns of DNA have been proven to cause cancer growth by repressing the expression of certain tumor suppressor genes. Twenty five percent of acute myeloid leukemia cases are linked to abnormal activity of the DNA methyltransferase 3a (DNMT3a), an enzyme responsible for the installation of methyl groups on the DNA. Currently, the only two FDA approved drugs that target the DNMTs are *Vidaza* and *Dacogen*, two highly cytotoxic compounds with poor pharmacokinetic profiles. There is an urgent need for alternative DNMT inhibitors, but their development is hampered by a high rate of false positives. To overcome this issue, we first established a sequence of biophysical and biochemical methods for the validation of hits against DNMT3a. This triage process led to the validation of a hit obtained through an AI-assisted virtual screen. A SAR study performed on the latter resulted in the development of AMP-226, a compound displaying a 6-foldpotency increase compared to the original hit. Furthermore, our methodology was applied to multiple hits from the literature, which allowed the validation of one compound originating from a virtual screening campaign. Taken together, these results suggest that these confirmed hits could serve as starting points for future hit-to-lead campaigns.

Synthesis and Mechanistic Insights into the Formation of 1,2-Bisphenylhydrazones

D. Patel*, I. Charley, D. Duncan

Brock University

1,2-Bisphenylhydrazones (BPHZs) are valuable scaffolds with applications in medicinal chemistry, materials science, and as intermediates in the synthesis of heterocycles. Conventional synthetic methods typically rely on1,2-dicarbonyl precursors, which are often difficult to access and limit structural diversity. In this study, we investigate an alternative and potentially more efficient route to substituted BPHZs through modified hydrazone condensation reactions using readily accessible ketoamides and substituted phenylhydrazines. Preliminary observations revealed the spontaneous formation of BPHZ species during hydrazone synthesis, prompting a systematic investigation into the reaction conditions and mechanism. The work involves optimizing stoichiometric ratios, solvent systems, and substitution patterns to identify parameters that promote BPHZ formation. This approach aims to establish a general, tunable, and mechanistically distinct method for accessing structurally diverse BPHZ frameworks from simple and readily available precursors.

Enantioselective Organocatalytic Synthesis of a [6-5-3] Tricyclic System via a One-Pot Tandem Sequence

C. Rocq*, S. Canesi

Université du Québec à Montréal

Organocatalysis, which was awarded the Nobel Prize in 2021, still has much to teach us. This highly valued form of catalysis in green chemistry enables the production of asymmetric systems using small, low-toxicity or non-toxic organic molecules as catalysts. These robust tools operate via different activation modes, tolerate a wide range of reaction conditions, and offer remarkable selectivity.

Here we describe a methodology for the efficient formation of an enantioselective [6-5-3] tricyclic system from a prochiral dienone that contains an aldehyde in its lateral chain. In the presence of an electrophilic halogen source and a diarylprolinol silyl ether organocatalyst (Jorgensen's reagent), cyclopropane formation is achieved in good to excellent enantiomeric excess through a one-pot, three-step reaction sequence involving α-iodination of an aldehyde, enantioselective Michael addition, and subsequent nucleophilic substitution.

After optimization, this amino catalysis approach provides excellent stereoselectivity and works on various substrates under mild conditions. Furthermore, these organocatalysts are simple, inexpensive, and readily available. This work aligns well with the current development of green chemistry, which promotes metal-free catalysis and more sustainable reaction conditions.

Cross-couplings of transiently stable organolithium compounds

P. Saha*, F. J. A. Troyano

University of Ottawa

Organolithium compounds are amongst the most important organometallic reagents and frequently used in difficult metalation reactions. Despite their importance, their direct use as nucleophiles in cross-coupling reactions to form C—C bonds are less common. Over the past decade, the Feringa lab have made significant advancements in the field of organolithium cross-couplings, primarily using commercial and/or stable organolithiums. The use of more complex organolithium compounds such as heterocycles remains largely unexplored, likely due to the poor lifetime of such molecules compared to the timescale of common cross-coupling reactions. This project aims to combine the concepts of flash chemistry to generate transiently stable organolithium species in continuous-flow systems and use them as nucleophilic partners in cross-couplings. High throughput experimentation was used to identify the optimal catalyst-ligand systems that enables these fast Murahashi-couplings to be carried out in minutes at temperatures as low as -30oC, expanding the opportunity of using a variety of organolithiums. The present research describes our effort towards using this novel catalyst system to successfully cross-couple transiently stable organolithiums faster than they decompose, with the goal of rendering the Murahashi coupling as an attractive alternative to coupling with organoboron and organozinc reagents, whose syntheses often proceeds via organolithiums.

Chemistry Education

Transforming Chemistry Education Through Interdisciplinary Training: Pathways for Future Scientists

S. Al Akkad*, A. Flynn

University of Ottawa

Chemistry is central to address global challenges in energy, health, and sustainability, all of which demand interdisciplinary collaboration. Yet, little is known about how best to train graduate students and postdoctoral researchers for such environments. In Canada, this need aligns with a diverse, multilingual graduate student population. As employers increasingly value transferable skills, graduate programs must provide integrative and inclusive training. However, many chemistry programs remain monodisciplinary, offering limited opportunities for collaborative or interdisciplinary learning that are vital for diverse career paths.

This study examines how advanced interdisciplinary training within chemistry can be optimized to foster knowledge integration, skills development, equity, and enhance career readiness. Adopting a mixed-methods research design, the core of the study will use a case study approach involving document analysis, interviews, focus groups, and observations of the program events and activities. To complement this, national surveys of graduate chemistry students and interviews with STEMM department heads, program coordinators, and employers will provide broader insights.

At this stage of the ongoing research, this presentation will outline the study's research questions, theoretical frameworks, design, and anticipated contributions. The goal is to spark dialogue and receive feedback from scholars involved in STEMM education reform and interdisciplinary program development.

The impact of using generative artificial intelligence on critical thinking and scientific reasoning in organic chemistry education

L. Temple-Murray*, A. B. Flynn

University of Ottawa

Over the past five years, educational institutions have continually adapted teaching and learning methods to incorporate emerging technologies. The release of generative artificial intelligence (GenAI) tools such as ChatGPT in 2022 further disrupted traditional learning by changing how students access information and complete tasks. While GenAI supports personalized learning through real-time feedback and adaptive interaction, questions arise about its impacts on users' metacognitive processes. Research suggests that reliance on chatbots for thinking tasks may reduce independent reasoning ability.

Our study investigates how undergraduate students at the University of Ottawa solve organic chemistry problems and construct scientific arguments with and without GenAI. For one problem, participants were randomly assigned to use either ChatGPT or a CustomGPT designed to promote metacognition. Their responses were thematically analyzed. Students were also surveyed on their perceptions of GenAI, prior use, and demographic affiliations related to language and academic background.

This presentation outlines the study design and preliminary findings on ChatGPT's impact on scientific argumentation and critical thinking. The efficacy of the metacognitive chatbot will also be discussed. Overall, this research will help guide effective use of GenAI for learning by showing how students engage with AI tools and how this shapes their reasoning and understanding.

Environmental Chemistry

Biosurfactant Based Micellar-Enhanced Ultrafiltration (MEUF) for Metal Recovery fromAlkaline Leachates

L. Cisneros*, C. Mulligan

Concordia university

The mining, metallurgical, and refining sectors generate large volumes of alkaline residues that can release metals into surrounding soil and groundwater, posing long-term environmental risks. Treating and recovering metals from such effluents remains a major sustainability challenge, as current methods rely on chemical reagents that produce secondary sludge and hinder metal recovery. Developing biosurfactant-based, circular processes that function under highly alkaline conditions has not yet been explored.

This study proposes a biosurfactant-assisted Micellar-Enhanced Ultrafiltration (MEUF) process using rhamnolipids and sophorolipids to enhance micelle formation and metal recovery. Metallurgical residues from an active iron and titanium industry in Québec will be used to generate controlled leachates characterized by high alkalinity and containing metals such as Ni, Cu, Zn, and Co. The MEUF system will employ hollow fiber ultrafiltration membranes to assess metal–biosurfactant interactions and membrane performance under varying pH and biosurfactant concentrations.

The proposed process aims to recover both metals and biosurfactants, supporting circular treatment strategies and contributing to sustainable remediation technologies. This research aligns with Canada’s Critical Minerals Strategy, which prioritizes the recovery of nickel, cobalt, copper, and zinc essential for clean energy technologies.

Integrating Organic Waste Oxidation as a Pathway for Hydrogen Production from Wastewater

T. Delesa*, F. Perreault

University of Quebec in Montreal

Hydrogen has emerged as a promising alternative energy source, with water electrolysis standing out as a clean method for its production. Electrochemical water splitting has gained attention due to its potential to supply green energy. However, commercial alkaline water electrolysis faces challenges, primarily due to the energy-intensive nature of the anodic oxygen evolution reaction (OER), which is characterized by high overpotentials. To address these, the electro-oxidation of organic substrates in wastewater is an attractive alternative to the OER. This approach mitigates the energy-intensive drawbacks of water electrolysis and provides a dual solution to two critical global challenges: waste management and sustainable energy production. This research explores the potential of organic waste oxidation as electron donor to enhance hydrogen generation from wastewater. By quantifying hydrogen output through gas volume analysis and current measurements, the study investigates the influence of varying concentrations of organic components on hydrogen production efficiency. A key focus is to identify the minimum threshold of oxidizable organics required for optimal hydrogen yield, to evaluate how this threshold varies across different organic molecules (such as urea, lignin, and glucose), and to advance the understanding of organic waste-driven hydrogen production while transforming wastewater into a viable source of clean energy.

Influence of additives on the adsorption of contaminants by microplastics: role of surface properties

D. R. B. Doussiemo*, F. Perreault

Université du Quebec à Montréal

Plastic waste released into the environment undergoes progressive degradation due to UV rays, wind, mechanical abrasion, and wave action. This fragmentation generates particles smaller than 5 mm, commonly referred to as microplastics (MP). These microplastics, due to their high surface area to volume ratio and hydrophobic nature, adsorb contaminants present in water and thus become vectors for various pollutants. During their manufacture, additives are incorporated into polymers to confer specific properties. These additives modify the structure of plastics, which is likely to affect their sorption capacity. However, most studies focus on the leaching of these additives and their toxicological effects. Our study therefore aims to evaluate the influence of the additive composition of microplastics on their capacity to adsorb environmental contaminants. To do this, we incorporated carbon black and glass fibers into a polyethylene matrix. We quantified key parameters influencing adsorption (hydrophobicity, crystallinity, surface area), then measured the adsorption of different contaminants. The results demonstrate the crucial role of additives on the surface properties of MPs and their interactions with contaminants, highlighting that their composition is a key factor in their ability to act as pollution vectors.

Biogeochemical Characterization and Source Prediction of Organic Matter in a Land to Ocean Sediment Transect by Multivariate Analyses and Machine Learning

Y. Mirzaei1*, C. Skinner2, G. Kos2, Y. Gélinas1

[1]Geotop Research Center and Concordia University, [2]Concordia University

Studying buried Organic Matter's (OM) origin, composition and fate in sediments is vital for comprehending the Earth's archival records, ecosystem dynamics, and impact of land inputs in marine systems. Limited number of samples, complexity of the matrix, and multiple biogeochemical properties, can all challenge OM source apportionments in its altered and degraded form. To overcome these limitations, this study applied multivariant analyses and machine learning techniques on all the biogeochemical properties of more stabilized OM in sediment samples, from the most terrestrially to marine affected stations. The land to ocean sediment transect of the St. Lawrence Estuary and Gulf was chosen as a natural reactor for input and burial of OM. We investigated the biogeochemical characteristics of sedimentary OM by measuring the biomarkers distributions (C17-C27 *n*-alkanes), elemental concentrations (C and N), and both bulk and compound specific stable carbon isotope values. Correlations of different variables among themselves and with OM sources were deconvoluted, with molecular and isotopic compositions standing out as strongest OM source tracers. Predicted values showed how terrestrial inputs and marine primary productivity changes along the system. This approach provides information on OM transportation/transformation, advancing our ability to study multiple variables in limites samples from natural systems.

Compilation and assessment of chemicals used in large quantities in Africa: Temporal trend-based prioritization and environmental risk characterization indicate urgent management and regulatory needs.

R. B. Opoku*, X. Zhang

Concordia University

The global chemical industry encompasses over 350,000 commercial substances, many of which are traded internationally through expanding global supply chains, making the movement of chemicals across borders a

key driver of environmental exposure worldwide. Industrialized regions including North America, Europe, East Asia, and Oceania have chemical inventories, but Africa's data coverage, assessments, and regulatory systems are limited. To address this knowledge gap, we compiled annual chemical trade data for all 54 African countries from 1996 to 2024, covering five chemical classes defined by six-digit Harmonized System (HS) codes. Each class, representing multiple individual chemicals, was analyzed using temporal trend clustering to identify rapidly increasing classes, which were then ranked by their 2024 trade quantities. To enable hazard quantifications, individual chemicals (CAS registry numbers and SMILES structures) within each class were extracted from the PubChem and EPI Suite databases and assessed for persistence, bioaccumulation potential, mobility, and toxicity using an in-silico approach. The resulting hazard ranges and relative environmental risks based on quantities of the chemicals will support a systematic framework to identify priority chemicals needing regulatory action. We propose cost-effective, practical measures that can be adopted by African nations for robust and proactive environmental risk management from commercial chemicals.

Analysis of micro/nanoplastics using fluorescent probe

F. Perreault, k. hamzi*

UQAM

Pollution by micro/nanoplastics (MNPs) is a major environmental issue, particularly in aquatic ecosystems where these particles can interact with various contaminants and affect marine fauna. Their detection remains a challenge due to their small size and dispersion in the environment, requiring sensitive and efficient analytical methods. This study explores the use of the fluorescent probe DCVJ (9-(2,2-Dicyanovinyl)julolidine) as an innovative tool to detect and quantify MNPs in aqueous media. This fluorescent molecule interacts with MNP sand emits a measurable light signal, allowing rapid and accurate detection. Unlike conventional methods, which are often complex and expensive (SEM, FTIR, Raman), fluorescence has the advantage of being faster, less invasive and suitable for real-time analyses. Initial results show a strong correlation between fluorescence intensity and MNP concentration, indicating a high sensitivity of the DCVJ probe. In addition, several parameters influencing this fluorescence are being evaluated, including particle size and the chemical nature of plastics. The objective is to optimize this approach to ensure reliable quantification of MNPs in various water samples. Ultimately, this method could be integrated into environmental monitoring strategies to better understand the dispersion of micro/nanoplastics.

Physical Chemistry

Novel Doping Agents for Degradation-Assisted Doping of Organic Semiconductors

M. Berteau-Rainville[1], T. P. L. Cosby[2], S. Bhagat[3], A. E. Laturski[2], M. Creran[3]*, E. Orgiu[1], T. Baumgartner[2], C. B. Caputo[2], I. Salzmann[3]

[1]Institut national de la recherche scientifique (INRS), [2]York University, [3]Concordia University

Introducing molecular dopants into organic semiconductors is essential to create high-performing organic electronics to complement and compete with their inorganic counterparts. As of recent, we have discovered through theory and experiment, the highly efficient doping mechanism we call degradation assisted doping(DAD) by using the prototypical, p-doping Lewis acid tris(pentafluorophenyl) borane (BCF) with the model semiconducting poly(3-hexylthiophene) (P3HT). We were further able to enhance the doping by introducing the radical trap, 2,2,6,6- tetramethylpiperidine-N-oxyl (TEMPO) which alters the thermodynamic equilibrium of the DAD mechanism. Currently, BCF is the only dopant known to undergo DAD and was able to increase hole density by up to two orders of magnitude. Therefore, it is essential to investigate the further

possibilities this mechanism has to offer. Herein, we probe the use of new Lewis acid dopant molecules that also undergo DAD with P3HT, including the novel tris(pentafluorophenyl) gallium (GaCF). By exploiting other materials to manipulate the density of states, we gain further insight into this doping mechanism and how to optimize charge carrier densities in organic semiconductors.

Experimental Insights into the Fragmentation Mechanisms of Lignin-Derived Radical Cations: A Quantitative iPEPICO Study of 4-Ethylguaiacol and Eugenol

S. Gondarry

University of Ottawa

The unimolecular dissociation pathways of the 4-ethylguaiacol and eugenol radical cations were explored using imaging photoelectron photoion coincidence (iPEPICO) spectroscopy. Threshold photoelectron spectra (TPES)and breakdown diagrams were analyzed using the Rice– Ramsperger–Kassel–Marcus (RRKM) theory. 4-Ethylguaiacol loses a •CH3 group dominantly at low energies in dissociative ionization, consistent with our prior mass-analyzed ion kinetic energy (MIKE) study. Nonetheless, the discrepancy between the RRKM-fitted methyl-loss *E*0 of 1.88 eV and the previously determined theoretical value (2.15 eV) revealed a new reaction pathway involving sequential hydrogen shifts and structural rearrangements. The eugenol radical cation was found to dissociate by the loss of •CH3 and CH3OH, in agreement with MIKE results. However, the energy barriers derived from the RRKM analysis (1.64 eV and 1.51 eV) were significantly lower than previous computational reaction barriers of 2.63 eV and 3.21 eV, respectively, indicative of alternative, lower-energy, rearrangement fragmentation mechanisms, analogous to that of 4-ethylguaiacol. Furthermore, an additional fragment ion was observed at *m*/*z* 104. This study highlights the critical role of experimental techniques in validating and refining computational models and demonstrates how quantitative spectroscopic data can uncover previously unidentified reaction mechanisms.

Improving The Understanding of Isoprene Pyrolysis Using Threshold Photoelectron Spectroscopy

E. White Buenger*, P. Mayer

University of Ottawa

Isoprene (2-methyl-1,3-butadiene) is a reactive volatile substance of relevance in phytochemistry, atmospheric and industrial chemistry. A common fate of isoprene is burning, necessitating greater understanding of how isoprene reacts and the products that may be obtained under high temperature conditions. Threshold photoelectron spectroscopy (TPES) was employed to identify the products of the pyrolysis of isoprene in a SiC microreactor at 1400 °C. The experimentally derived mass-selected TPES (ms-TPES) were extracted and compared to Franck-Condon simulations for the identified molecular species.

A key observation from the ms-TPES of m/z 68 was equimolar amounts of isoprene and cyclopentene at this temperature indicating a kinetically competitive isomerization. This isomerization was computationally explored and was found to be consistent with literature findings that vinyl cyclopropane can decompose into both isoprene and cyclopentene, but the latter is the predominant reaction. Cyclopentene then decomposes by loss of H2 to form m/z 66, cyclopentadiene (also observed). Previously postulated products of dimethylallene, methylallene, and allene were not observed. The results draw into question a number of the suggested reaction products in the recent literature and thus the kinetic models used to map isoprene pyrolysis.

Biochemistry

Myxococcus-Based Elicitation Enhances Antimicrobial Biosynthesis in Aspergillus terreus

E. Ali*, B. Findlay

Concordia University

The rapid rise of antimicrobial resistance has created an urgent need for new antimicrobial compounds. Many microorganisms possess silent biosynthetic gene clusters (BGCs) that are not expressed under standard laboratory conditions, thereby limiting their potential for natural product discovery. In this study, we explored amicrobial elicitation strategy using lyophilized cells of the predatory bacterium *Myxococcus xanthus* to stimulate secondary metabolism in the saprotrophic fungus *Aspergillus terreus*. The underlying rationale is that chemical cues from *M. xanthus* cells mimic natural ecological interactions, thus activating cryptic biosynthetic pathways in *A. terreus*. Comparative LC-MS profiling of elicited versus non-elicited cultures revealed distinct metabolite peaks exclusive to the elicited samples. Subsequent antimicrobial assays demonstrated that several of the induced metabolites exhibited strong inhibitory activity against *Micrococcus luteus*, a Gram-positive bacterium. These findings highlight the effectiveness of our approach in unlocking cryptic microbial biosynthetic pathways and accelerating the discovery of novel antimicrobial drugs.

A capture-based approach for the separation of ligand-induced riboswitch conformations

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McGill University

Riboswitches are structured, non-coding RNA elements that bind specific ligands and undergo conformational rearrangements ("switching") to regulate downstream gene expression. The development of ligands that inhibit riboswitch switching presents a promising avenue for antibacterial drug discovery, but mutations within riboswitch sequences may restore switching competency. Currently, little is known about the impact of riboswitch sequence mutations on ligand binding, and consequently, if these would manifest as changes in riboswitch switching.

This presentation describes the development of a capture-based method to separate riboswitches according to their conformational states. Single-stranded DNA probes designed to detect specific riboswitch conformations were immobilized onto oligo d(T)25-functionalized magnetic beads, and these probe-conjugated beads enabled selective capture of riboswitches in defined ligand-induced conformations. The resulting conformations were pooled then amplified and quantified using RT-qPCR.

This capture-based method establishes a foundation for high-throughput screening of riboswitch mutation libraries to uncover key nucleotides involved in conformational switching, ultimately guiding the design of riboswitch switching inhibitors.

Synthesis and Characterization of C5-Modified Arabinonucleic Acids

S. Dao-Tse

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Arabinonucleic acid (ANA) is a chemically modified oligonucleotide capable of hybridizing with RNA, can support RNase H mediated degradation of RNA and resists nuclease degradation which are ideal properties for antisense oligonucleotide (ASO) therapeutic applications. Drawing from prior achievements involving C5-propynyl derivatives, we are now exploring the introduction of alternative modifications at the C5 position to

further enhance the properties of ANA. Synthesis of these ANA modifications involves protection of arabinouridine, iodination of the C5-position and palladium-catalyzed coupling of various groups to prepare phosphoramidite derivatives for solid-phase oligonucleotide synthesis. Biophysical characterization using UV thermal denaturation and circular dichroism will assess duplex stability and conformational effects, while RNase H activity assays will determine enzymatic degradation efficiency. Nuclease resistance studies will further evaluate the stability of modified oligonucleotides for applications in biological environments. By systematically analyzing these properties, this research aims to contribute to the development of chemically optimized ASOs with enhanced therapeutic potential for gene silencing applications.

RNA Aptamer-based Biosensing in Living Cells and Animals

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McGill University

There is a shortage of biosensors that are functional within living animals over their lifetime and multiple generations. Furthermore, many biosensors are invasive, limiting the ability to obtain real-time measurements. This is important when studying reactive oxygen species, which are critical for a range of processes, including but not limited to, biological and industrial processes. In this presentation, I introduce a non-invasive genetically encoded ‘RNA switch’ based biosensor to detect 8-oxo-guanosine triphosphate (8-oxo-GTP) and its metabolites. The RNA biosensor consists of an RNA aptamer that binds to oxidized guanine species. In this presentation, I will describe out work developing the biosensor and characterizing the kinetics, sensitivity, and specificity. This represents the first genetically encoded RNA biosensor for oxidative stress. We expect our sensor will enable the development of transgenic animals expressing our RNA-based sensors throughout their lifetime and for further generations. In addition, our biosensor will be utilized to address unanswered questions related to toxicology and disease pathology.

Insights into liquid-to-solid transitions of ultra-short peptides coacervates yield a new classof peptides that enable next-generation solvent-free catalysis

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McGill University

Ultra-short peptide coacervates (USPCs), formed via liquid–liquid phase separation (LLPS) of peptides with five or fewer amino acids, have emerged as promising systems for microreactors, drug delivery, and as models for understanding LLPS and liquid-to-solid transitions (LSTs) in biomolecular condensates. Their uniquely hydrophobic liquid interiors distinguish them from other coacervates, enabling previously challenging aqueous reactions. However, current USPCs lack long-term stability, undergoing LSTs within seconds to hours, which form fibers or gels and lose the hydrophobic liquid environment essential for their function. This instability limits practical applications and can cause adverse effects in biological systems. Here, we elucidate molecular principles that govern LLPS in USPCs and leverage these insights to design a new class of peptides with significantly enhanced resistance to LSTs without the need for additives or peptide mixtures. Increased stability enables slower, more complex photocatalytic and enzymatic reactions with water-insoluble catalysts, expanding the practical application scope of USPCs.

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

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McGill University

HalM2 is a model class II lanthipeptide biosynthetic enzyme, catalyzing post-translational modifications of theHalA2 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 15N labeled HalA2 is incubated with HalM2and 15N/1H 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 HalM2variant 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.

Size Matters: Reconstructing a Functional Tripartite Multidrug Efflux Pump in a Lipid Bilayer

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Tripartite multidrug efflux pumps are membrane protein complexes that export antibiotics out of bacterial cells and contribute to the emergent threat of antibiotic resistance. One pump in particular, MacAB-TolC, is implicated in tigecycline and macrolide resistance in the critical priority pathogen Acinetobacter baumannii. The dynamics and intricate assembly of this efflux pump are poorly understood, and the influence of the lipid bilayer on the mechanism of action and assembly has yet to be studied. To better understand the interactions between the different proteins making up this pump, we have engineered a fluorescence-based assay to monitor the transport of various substrates, utilizing reconstituted protein-lipid bilayer discs. Our study highlights the importance of the lipid bilayer on the action of this efflux pump, something that has yet to be done. These exciting findings elucidate dynamics of this tripartite efflux pump and the conformations that are necessary for proper functioning. Ultimately, understanding the different mechanisms that orchestrate this efflux pump, could allow us to predictand/or identify points of inhibition, bringing us a step closer to combatting antibiotic resistance.

Toward In Vivo Olefin Metathesis: Targeted Catalyst Delivery via a Protein-Catalyst Conjugate

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Olefin metathesis, as a versatile method for building carbon-carbon bonds, has enormous potential as a tool in chemical biology. At the frontier of such efforts is in vivo olefin metathesis, in which metathesis takes place within the living cell. Examples include ring-closing metathesis (RCM) in bacteria by a metalloenzyme containing biotinylated Ru, and, more recently, metathesis of unsaturated fatty acids in living algae for the production of olefins. A limitation in the latter goal is the reliance on passive, affinity-labelling means to transport the catalyst into the cellular compartments (the lipid droplets, LDs) in which the metathetical

production of 1-olefins is planned to occur. Poor specificity arising from diffusion of an affinity-tagged catalyst results in accumulation of catalyst in lipid-rich areas outside the LDs.

Here we describe a union of these approaches to enable *targeted* catalyst transport into the LDs. The catalyst is conjugated to the Major Lipid Droplet Protein, a protein which, as the name suggests, localizes to the LD. This approach is designed to improve metathesis productivity and reduce cell toxicity by limiting non-specific interactions, shielding the catalyst from the cellular environment during transport, and aiding catalyst localization/retention in the LD. Advances toward this goal will be described.

How Many Cytosines Must Be Protonated? Site-Specific Insights into i-Motif Folding from NMR and UV-Vis Studies

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McGill University

i-Motifs (iMs) are non-canonical DNA secondary structures formed in cytosine-rich sequences through hemiprotonated C–C base pairs in four intercalated cytosine tracts. Because cytosine has a pK_a of ~4.2, iMfolding typically requires acidic conditions, raising questions about their stability at physiological pH (~7.4). Despite this, iMs have been observed in vivo and implicated in gene regulation, although the mechanisms underlying their formation and stability remain poorly understood.

In this study, we investigate the relationship between cytosine protonation and iM stability. Using UV-Vis spectroscopy, we monitored the folded population of a highly stable iM across a range of pH values. Complementary NMR spectroscopy provided insight into both the folded state (via H1′ and aromatic proton resonances) and protonation state (via imino proton resonances directly involved in C–C base pairing). Our results show that cytosines deprotonate more readily than the iM unfolds, suggesting that iMs can persist even without full protonation of all cytosines in the C-tracts. To achieve site-specific resolution, we further employ isotope-labeled NMR to identify which cytosines are more or less prone to deprotonation, offering a nuanced view of how protonation heterogeneity contributes to iM stability near neutral pH.

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

T. Rutherford*, C. Wilds

Concordia University

O6-Alkylguanine DNA alkyl transferase (AGT) is a DNA repair protein capable of directly removing various alkyl adducts from the O6-atom of 2'-deoxyguanosine (dG). Our laboratory has previously demonstrated that hAGT can “unhook” intrastrand cross-linked (IaCL) DNA, where two adjacent dG residues lacking a phosphodiester linkage are covalently linked through their O6-atoms. Leveraging this activity as an endogenous stimulus, we designed a DNA tetrahedron (TDN) containing these IaCL at the vertices that could undergo disassembly by hAGT. Employing solid-phase synthesis, four complementary three-way junction (TWJ)oligonucleotides were prepared with IaCL of various alkylene chain lengths at each branch site. Denaturing PAGE analysis revealed that these TJW oligonucleotides assembled to form a stable TDN structure. Moreover, UV thermal denaturation experiments revealed that the thermal stability of the DNA TDN was not affected by the IaCL alkylene chain length. Future work will evaluate modifications to these IaCL containing TDNs for enhanced cellular uptake and therapeutic effect.

Harnessing Lipid Peroxidation for Photoactivatable Ferroptotic Cell Death

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McGill University

Photodynamic therapy (PDT) and ferroptosis each harness oxidative stress to kill cancer cells and have been gaining interest as a combined therapy for cancer treatment. Ferroptosis is a type of cell death characterized by runaway lipid peroxidation, but its kinetics and interplay with PDT, a treatment that uses a photosensitizer to kill cancer cells, remains a developing field. In this work, we used a fluorogenic radical trapping antioxidant (RTA) to quantify lipid peroxidation dynamics during RSL3-induced ferroptosis. The results were used to map the conditions for selective photoactivatable cell death with a dormant RTA photosensitizer. Our results allowed us to model real-time lipid peroxidation kinetics in ferroptosis, define the photosensitizer dependency on RSL3dose, and provide a framework to exploit lipid peroxidation for photoactivatable ferroptotic cell death.

Adaptive Evolution of *E. coli* Under Antibiotic Pressure Reveals Media Specific Patterns of Collateral Phenotypes

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Concordia University

Antibacterial susceptibility testing (AST) follows standardized guidelines to detect resistance and predict the clinical efficacy of antibiotic treatments. Cation-adjusted Mueller Hinton Broth (MHB) is routinely used as the reference medium to provide a controlled environment for bacterial growth and assessment of antibacterial activity. However, these guidelines and media formulations overlook the physiological conditions that influence in vivo antibiotic effectiveness.

Urinary tract infections (UTIs) are among the most prevalent bacterial infections, posing a major burden on healthcare systems and antibiotic use. In this study, nitrofurantoin-resistant *Escherichia coli* ATCC 25922mutants (n = 16) were developed using soft agar gradient evolution (SAGE) in two different media: MHB and artificial urine medium (AUM). SAGE establishes a continuous antibiotic gradient that enables gradual adaptation and resistance development.

AST of these mutants revealed higher minimum inhibitory concentrations in AUM than in MHB for nitrofurantoin, levofloxacin, and trimethoprim. Nitrofurantoin-resistant mutants evolved in MHB displayed collateral sensitivity, whereas those evolved in AUM exhibited cross-resistance. Moreover, AUM-evolved replicates showed medium-dependent differences in collateral phenotypes and significantly reduced fitness compared to MHB-evolved counterparts.

These findings underscore the importance of considering physiological conditions at infection sites when selecting media for MIC determination to improve the clinical relevance of susceptibility testing.

Synthesis of Oligonucleotide Conjugates Containing Selenium Modified Linkers

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Concordia university

Oligonucleotide conjugates are valuable nucleic acid modifications with therapeutic potential due to their ability to enhance cellular uptake, stability, and targeted delivery. These conjugates can involve small molecules like cholesterol or larger, complex structures such as peptides. However, their synthesis is often challenging due to chemical incompatibilities between ligation partners. Our laboratory recently developed a reductive diselenide–

selenoester ligation (rDSL) strategy to prepare DNA–peptide conjugates, employing a 5′-diselenide cross-linked DNA dimer and a C-terminal selenoester peptide for efficient coupling.

In this study, we synthesized alkylene linkers containing terminal 2-cyanoethyl-protected selenium for 5′-endcoupling to oligonucleotides. Phosphoramidite derivatives of tetra- and decamethylene linkers were prepared and incorporated into DNA on solid support. After deprotection, the longer linker formed a stable 5′-diselenide DNA dimer, confirmed by denaturing PAGE. This dimer was further functionalized by alkylation with different species, and the resulting products were analyzed by PAGE and mass spectrometry. Future work will explore extending this strategy to RNA and chemically modified oligonucleotides. Developing efficient selenium-based linker systems for oligonucleotide conjugation will enhance the synthesis of multifunctional nucleic acid conjugates and support their expanding use in therapeutic applications.

Novel Antimicrobials from Arctic Bacteria *Alteromondales*

A. Woodhead

Concordia University

Antimicrobial resistance (AMR) is an escalating global crisis projected to cause 10 million deaths annually by2050. The evolution of AMR far outpaces the discovery of new antimicrobial compounds, particularly against Gram-negative pathogens such as *Pseudomonas aeruginosa* and *Acinetobacter baumannii*. Although medicinal chemistry has optimized existing scaffolds, most clinically used antibiotics still originate from microbial natural products, largely from soil environments.

Discovery in new environments and organisms is often hindered by the repeated isolation of known compounds. While metagenomics can reveal uncharacterized biosynthetic gene clusters (BGCs), it does not confirm whether these metabolites are produced or active. A polyphasic chemical-ecology approach instead leverages microbial interactions and environmental context to identify promising leads.

This study investigates ribosomally synthesized and post-translationally modified peptides (RiPPs) from Canada's Arctic Ocean (*Ualiniup Tariunga*) as a potential new subclass of antimicrobial compounds. Clustering analyses show Arctic RiPP BGCs are phylogenetically distinct from known clusters. One RiPP BGC is shared across several families of *Alteromonadales*, including algae-associated sea-ice species. The structure and Gram-negative bioactivity of this RiPP group is shown, providing a novel compound for drug scaffolds and highlighting Arctic sea-ice microbiomes as a heterogeneous habitat- not dissimilar to soils, where secondary metabolites plays an outsized role.

Inorganic Chemistry

Hard single-molecule magnet behavior and strong magnetic coupling in pyrazinyl radical-bridged lanthanide metallocenes

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Contemporary lifestyle is interwoven with technological achievements that implement the use of permanent magnets. Polynuclear lanthanide single-molecule magnets (SMMs) lack strong magnetic communication, which renders the design of high-performing SMMs an ongoing challenge. To overcome this, incorporation of radical pyrazine (pyz·−) linkers between lanthanides is a compelling approach. Careful tuning of the synthetic conditions led to dinuclear [(Cp∗2LnIII)2(pyz·−)(THF)2][BPh4] (Ln = Gd (**1**), Dy (**2**); Cp∗ =

pentamethylcyclopentadienyl; THF = tetrahydrofuran) and tetranuclear [(Cp∗2LnIII)4(pyz·−)4]·10THF (Ln = Gd(**3**), Dy (**4**)) complexes. Magnetic and computational studies reveal one of the highest exchange couplings (*J*Gd-pyz = −22.2 cm−1) for a radical-bridged system, achieved by two 4*f*-SOMO interactions. This, combined with the significant anisotropy of the DyIII, grants **2** and **4** with slow magnetic relaxation at zero field and open hysteresis loops. A giant coercive field of 65 kOe renders **4** as the hardest radical-bridged Dy-based SMM.

Evaluating Structure/Activity Relationship of Heteroleptic Copper (I)-Based Complexes

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A library of heteroleptic copper(I) photocatalysts were prepared and evaluated in Minisci-type reactions using blue light to try and elucidate important structure-activity relationships. Three biphosphines, one NHC and five diimines comprised the ligand library, and were selected to gain insight into the roles of bite angle, electron-donating and withdrawing substituents and extended conjugation on redox properties and photostability of the resulting complexes. The study presents important insight on the development of sustainable catalysts for synthetic photochemistry.

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

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Concordia University

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

Size and Ligand Effects on Ru Nanoparticles for Hydrogen Evolution

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In recent years metallic nanoparticles (NPs) have increased their popularity for numerous catalytic applications. One particularly interesting method for the synthesis of metallic NPs is the organometallic approach. This procedure entails the controlled decomposition of an organometallic precursor in the presence of a stabiliser, usually a ligand of interest, under mild conditions. In this way, the synthesised NPs present a clean surface free of contaminant by-products. Interestingly, the ligands attached to the surface of NPs have been shown to alter the physicochemical properties of the system and even increase their catalytic efficiency, similarly to organometallic complexes. Herein we present various systems consisting of Ru NPs stabilised with

different amounts of 2,2'-bipyridine (bpy). It was found that there is an inverse relationship between the amount of bpy used and the NP size. These differences in size also translate into their catalytic performances towards hydrogen evolution, being the smallest system the worst and the largest one the best. This behaviour can be justified by the effect of the bpy ligand on the active sites of the NPs by a combination of experimental (electrochemistry, XPS,XAS) and computational studies.

A Systematic Study on the Molecular Symmetry and Magneto-Optical Behavior of Lanthanide(III) Complexes: Implications for Magnetic Circularly Polarized Luminescence

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Lanthanide (III) materials exhibit exceptional optical properties, including sharp emissions and long lifetimes, which are sensitive to external factors such as temperature and magnetic fields. Among the various stimulus-responsive phenomena, the magnetic effect of transition polarization opens new horizons to explore magneto-optical techniques like magnetic circularly polarized luminescence (MCPL), which is a powerful method that relies on the differential absorption of right and left circularly polarized light. On the other hand, the geometry around the lanthanide can be tuned with the choice of ligand, opening plenty of room for new material design. Furthermore, their impact on magneto-optical properties is yet to be explored and could be the way to understand the structure-luminescence relationship.

In this study, we investigate a series of Eu (III) complexes with systematically varied substituents. These structural variations alter the ligand-field environment, influencing electronic transitions. Additionally, by applying magnetic fields, spin degeneracy is lifted via the Zeeman effect, further modulating transition probabilities. A detailed magneto-optical study has been performed to understand the structural correlation with lanthanide luminescence and their sensitization. These insights are expected to reveal design principles of such highly luminescent lanthanide complexes, which hold potential for future applications such as thermometry and barcoding.

Highly efficient and photostable Ruthenium terpyridine complexes as photosensitizers for artificial photosynthesis

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The recent climate crisis has focussed attention on the need for green and affordable energy; however, many avenues are available to produce green energy. One of the most promising ways is the photocatalyzed production of hydrogen, as sunlight is the most abundant and widely available energy source on Earth. Our first target is a novel molecular platform to harness energy emitted from the sun. Thus, a polytopic tridentate polypyridine-based ligand bearing three exterior pyridyl moieties, 4,4',4''-tris(4'''-pyridyl)-2,2':6',2''-terpyridine (Py3Tpy), allows for facile electron transfer to appended cobalt catalysts to complete the Hydrogen Evolution Reaction (HER). Py3Tpy coupled with an electron-donating terpyridine yields highly stable and ruthenium heteroleptic complexes with exceptional hydrogen production (Figure). We present herein three new Ru(II) complexes as well as their incredible results in the HER surpassing any ruthenium-based photosensitizer in the current literature.

Iron Coordination Complexes as Aqueous Electrolytes for Redox Flow Battery Applications

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Concordia University

The world requires reliable and renewable energy alternatives to fossil fuels. However, since most renewable energies will not supply continuous power, it is imperative to have clean energy storage methods. Grid-scale electrochemical energy storage technologies such as redox flow batteries (RFBs) are of interest because they offer a low-cost and sustainable option. The energy in flow batteries is stored within redox active electrolytes, that flow through the battery. Therefore, of particular focus are the selection of electrolytes and their respective solvents. To date, diverse electrolytes composed of metal-ligand coordination complexes dissolved in aqueous salt solutions have been explored, where the electrolytes in both half-cells must be electrochemically compatible to be employed together in the battery.

This work discusses the synthesis and characterization of iron$^{2+/3+}$ ethylenediaminetetraacetic acid (EDTA) and iron$^{2+/3+}$ polypyridine complexes, as aqueous electrolytes in redox flow batteries. Preliminary characterization of these iron-based electrolytes includes infrared and optical spectroscopies, optical microscopy, Pourbaix analyses and ground state electrochemistry. Additionally, the stability of these electrolytes was evaluated via symmetric cell cycling (under an inert atmosphere), where capacity fade rates as low as 0.13 % per day were obtained for the $[Fe^{2+/3+}(EDTA)]^{2-/-}$ electrolyte.

A bright exception: Spectroscopic rationale of anti-Kasha photophysics of Co(III)-Amidine-N-Oxide complexes

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The photophysical properties of 3d metal complexes remain a fascinating field of study, particularly when transitioning from the rare 2nd and 3rd row metal complexes towards their 1st row congeners. Here, we present two novel photoactive Co(III) metal complexes based on amidine-*N*-oxide ligands. These complexes exhibit unusual anti-Kasha type singlet emissions. Contrary to the widely accepted Kasha emitters which emit from the lowest-lying excited state, these complexes show room temperature fluorescence from higher-lying states consisting of an admixture of ^{1}p-p* and intra-ligand charge-transfer (^{1}ILCT) character. Detailed steady state and ultrafast spectroscopy alongside extensive theoretical calculations establish the electronic factors governing this behavior. The structural rigidity and higher-lying p orbitals of the ligands render these metal complexes photoactive.

Synthesis and study of single molecule magnetic behaviour in lanthanide metallocene complexes with 3,6-bis(3-pyridyl)tetrazine radical

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Single-molecule magnets (SMMs) exhibit magnet-like behavior and show slow relaxation of the magnetization of purely molecular origin, making them promising candidates for applications in high-density data storage. However, promoting strong magnetic interactions in lanthanide-based SMMs remains an ongoing challenge due to the core-like nature of the 4f orbitals, which prevents the coupling between the lanthanide ions. Incorporating paramagnetic bridging ligands has emerged as an effective strategy to mediate stronger magnetic interactions by promoting direct exchange between lanthanide ions.

1,2,4,5-Tetrazines or s-tetrazines are ideal scaffolds for ligand design due to their strong electron-accepting properties, redox activity, and the exceptional synthetic tunability. Building on these features, we aimed to investigate pyridyl substituted s-tetrazines, namely, 3,6-bis(3-pyridyl)tetrazine (bptz), a rigid, redox-active, and conjugated framework capable of binding through bridging and/or chelating modes creating multiple coordination sites. Using these properties, we incorporated bptz into lanthanide metallocenes, leading to the formation of tetranuclear $[(Cp^*_2Dy)_4(bptz^{\cdot-})_2(bptz)_2][(BPh_4)_2]\cdot 10THF$ (**1**) (Cp^* = pentamethylcyclopentadienyl, THF = tetrahydrofuran) and dinuclear $[(Cp^*_2Dy)_2(bptz)(THF)_2][(BPh_2)_2]\cdot 2THF$ (**2**) complexes. These represent the first lanthanide metallocene complexes featuring the bptz ligand. Magnetic investigations of **1** revealed zero-field single-molecule magnet behavior, demonstrating the potential of bptz as a bridging ligand for enhancing magnetic communication in lanthanides.

Thiol-Functionalized Metal–Organic Frameworks as Drug Delivery Platforms for Ophthalmic Therapeutics

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Cataracts are an ophthalmic disease characterized by clouding in the eye's lens. The treatment generally involves the surgical replacement of the natural lens with clear artificial ones. After surgery, non-steroidal anti-inflammatory drugs (NSAIDs) such as flurbiprofen are commonly prescribed to reduce inflammation. These medications are administered as ophthalmic drops, which are a standard route for ocular drug delivery. This drug delivery protocol often suffers from low drug bioavailability due to the poor mucoadhesion of current formulations.

Metal–organic frameworks (MOFs) are an interesting platform that are underexplored for ophthalmic drug delivery applications, and specifically as mucoadhesive drug vectors. MOFs are porous materials comprised of metal nodes bridged by organic linkers. Their syntheses are highly modular and often yield crystalline solids with high surface areas. One strategy that can be used to improve the mucoadhesive properties is functionalization with thiol groups (–SH). Thiol groups can interact with the amino acids present on the mucin glycoproteins, thereby improving the retention time of these drug carriers at mucosal surfaces. Herein, thiol-functionalized Zr-MOFs (UiO-66-$(SH)_2$ and UiO-67-$(SH)_2$) were synthesized and characterized. Their mucoadhesive properties were assessed, and the encapsulation and release of flurbiprofen by Zr-UiO-66-$(SH)_2$ and Zr-UiO-67-$(SH)_2$ were evaluated and compared with non-functionalized samples.

Analytical Chemistry

Instrument Development for Targeted Heart-Cuts of Complex Samples from a Sheath-Flow-Interface Capillary Electrophoresis Array

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Capillary electrophoresis (CE) high separation efficiency makes it an ideal choice for challenging biological separation. The limited sample injection volume (~1000's pL) hinders secondary analysis (eg. MS). Heart-cutting, a strategy in which a segment of the electropherogram is captured onto a secondary capillary, reduces the complexity of the electropherogram and provides an opportunity for further manipulation such as collection. Given the minute sample volume, and large dilution factor of the outlet vial, practical heart-cutting CE is limited to high abundance species. Current CE heart-cutting interfaces are limited to one heart-cut per separation. This requires multiple sequential heart-cuts to deposit enough low abundance analytes in the outlet vial,

reducing throughput and increasing operational costs. Here we demonstrate a novel instrument which can perform parallel heart-cuts to both number-up the collected sample and minimize sequential runs. A custom-built sheath-flow-interface allows for 5 parallel CE separations using a common separation voltage to carry out the initial high-resolution separation. All heart-cuts are consolidated onto the single capillary, the outlet of which can be used for direct on-line detection. The sequential capture of a target peaks across the capillary array for detection of low abundance, and partially resolved, biological analytes is currently being explored.

Determination of the pyrolysis products and decomposition mechanisms of per/polyfluorinated compounds using imaging photoelectron photoion coincidence spectroscopy (iPEPICO)

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The strong C-F bond found in per- and polyfluorinated compounds (PFCs) enables them to resist degradation and remain persistent in the environment. To remove PFCs from the environment, thermal treatment is often preferred, but research shows that incomplete degradation occurs. This creates small and volatile fluorinated compounds that can impact the environment. To investigate this, three short-chain PFCs, 2,2,3,3,3-pentafluoropropionic acid (**1**), 3,3,3-trifluoropropionic acid (**2**), and 2,2,3,3,3-pentafluoro-1-propanol (**3**), underwent pyrolysis in a Chen-type microreactor under dilute conditions. The products were ionized with VUV synchrotron radiation at the Swiss Light Source and identified by their mass-selected threshold photoelectron spectra (ms-TPES). The results are compared to calculated TPES from Franck-Condon simulations preformed at the B3LYP/6-311+G(d,p) level of theory. **1** produced 1,1-difluoroethylene, carbon dioxide, difluoromethylene, and formaldehyde. **2** produced 2,2,2-trifluoroethanol, 1,1-difluoroethylene, difluoromethylene, carbon dioxide, formaldehyde, carbon monoxide, and acetylene. **3** produced trifluoroethene, 1,1-difluoroethylene, difluoromethylene, and formaldehyde. The reaction pathways forming the products were then determined for all three molecules.

Computational Chemistry

Computational Investigation of Reaction Mechanisms in Pd-, Ni-, and Au-Catalyzed Systems

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McGill University

Understanding catalytic reaction mechanisms is fundamental to improving selectivity and efficiency in chemical reactions. We performed density functional theory (DFT) calculations on a series of experimentally developed catalytic systems to validate proposed mechanisms and clarify the factors governing rate and selectivity. For a Pd-catalyzed three-component Heck–Tsuji reaction involving aryl halides, allenes, and hydrazones, DFT reproduces the catalytic cycles and explains the observed regiodivergence, showing how ligand-dependent coordination environments determine product distribution. In a Ni-catalyzed coupling of allylic alcohols with carbonyl derivatives, computed free energy profiles and kinetic simulations validate the proposed pathway and show that the branched product is kinetically favored, consistent with experimental selectivity. For a Ni-catalyzed methylation using formaldehyde hydrazone, calculations confirm that C–C bond formation occurs through a pathway with a lower barrier than the competing route leading to C–N coupling, explaining the observed selectivity. Finally, for an Au-catalyzed intramolecular hydroamination of an allene, calculations reveal that the rate enhancement observed with ligands containing a P=O group originates from a stabilizing intramolecular hydrogen bond between the allene and the P=O moiety, which lowers the activation barrier and

increases the reaction rate. These computational studies bridge experiment and theory, providing a unified mechanistic understanding across transition metal catalysis.

Theoretical investigation of *para*- and *ortho*-water reacting with C^+ and CO^+ ions in the interstellar medium

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Water (H_2O) plays a central role in both terrestrial life and the chemistry of the interstellar medium (ISM). Water exists as two nuclear spin isomers, *para*- (p-H_2O, I = 0) and *ortho*-water (o-H_2O, I = 1)—that exhibit distinct physical properties. Whether these differences also affect chemical reactivity under astrochemical conditions remains an open question. This work explores the reactivity of p- and o-H_2O with C^+ and CO^+ ions, combining ab initio calculations, rotationally adiabatic capture theory, and simulations with the Nautilus astrochemical model. Reaction rate coefficients were calculated and implemented into ISM models of diffuse clouds. The reactions $C^+ + H_2O$ and $CO^+ + H_2O$ were confirmed to yield HCO^+ and HOC^+, with p-H_2O consistently showing a greater reactivity. However, despite these kinetic differences, no significant variations in the modeled abundances of H_2O, C^+, CO^+, HCO^+, or HOC^+ were observed. These results suggest that while spin isomerism influences reactivity at the molecular scale, its effect on macroscopic interstellar abundances is limited. This analysis provides new insight into the role of how rotational-state-specific reactivity impacts the molecular composition of different interstellar environments.

Development and Evaluation of Machine Learning Models to Screen Environmental Risks of Chemical Features Based on Information Gained from Non-targeted Chromatography-Mass Spectrometry Analysis

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Mass spectrometry (MS) is a powerful tool for detecting and analyzing chemicals in complex environmental samples, but interpreting raw mass spectra for environmental risk assessments remains challenging. To address this, machine learning (ML) can give practical tools for modeling complex data. In this study, we used ML to predict environmental impact based on MS data, which provides detailed chemical profiles without identifying specific compounds. We developed and evaluated classification models to predict bioaccumulation, toxicity, and persistence to connect MS data to environmental chemical endpoints. Through hyperparameter tuning and 10-fold cross-validation, the models demonstrated strong predictive performance, achieving an accuracy of over 0.9on test sets. No significant difference (< 7 %) between the test and training results suggests that the models are well-generalized. For all models, the fractions corresponding to the mass-to-charge ratios (m/z) of M+2, M+4, M+5, and M-70 were found to have a significant impact on the model's ability for classification and prediction. Some of these fractions may be linked to halogens, known for their distinct isotopic patterns and environmental risks. This work demonstrates how ML models can link MS data to chemical risk assessment, which enables ecological predictions even in the absence of complete structural information.

Machine Learning QSAR Modeling for Cannabinoids & the CB1/2 Receptors

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Phytocannabinoids are a class of chemicals found in the Cannabaceae family and have been shown to interact with the Endocannabinoid System (ECS). The ECS is responsible for inflammation, immune responses, appetite, pain-sensation, memory and more, primarily through modulation of the Cannabinoid 1 and 2 receptors (CB1 &CB2). The goal of the study is to better understand how minor cannabinoids interact with the human cannabinoid receptors using in silico modelling to establish patterns based on compound structure. Relative affinities of 200+cannabinoids were accomplished using Autodock Vina (docking software). Four receptor models were chosen for CB1 and CB2, both in active and inactive conformations. The active sites and molecular interactions were explored using PyMol molecular visualisation software. QSAR parameters included factors such as compound chain length, molecular weight, number of rotatable bonds, number of hydrogen bond donors & acceptors as well as interaction bond length and type of bond formed. Pharmacokinetics were predicted using SwissADME and subsequently factored into a machine learning QSAR model. Preliminary results show certain structural patterns influence affinity. Next steps include step wise modification of structures and testing in silico for potential lead.

Molecular Biology

Vacuolar pH regulates clathrin-mediated endocytosis through TORC1 signaling during replicative aging

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Clathrin-mediated endocytosis (CME) is a critical cellular process that regulates nutrient uptake, membrane composition, and signalling. Although replicative aging affects many cellular functions, its impact on CME remains largely unknown. We show that in budding yeast, older cells have slower assembly of early and coat CME modules, resulting in longer endocytic turnover and reduced Mup1 internalization. This change in CME dynamics is mother cell-specific, and not observed in daughters. Our data also show that perturbing vacuolar pH, a key driver of aging phenotypes, in young cells mimics aging-like CME dynamics, while maintaining an acidic vacuolar pH in aging cells preserves CME dynamics typical of young cells. We demonstrate that the vacuolar pH effect on CME is regulated through TORC1 via the effector kinase Npr1. Finally, we show that rescuing CME in aging cells improves mitochondrial health. These findings reveal that age-associated changes in cellular and vacuolar pH impair CME, and suggest CME as a potential driver of early cellular aging. (Presentation will be in English).

Spatiotemporal silencing of mRNAs during hibernation: Roles of stress granules and P-bodies

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Hibernation is an extreme physiological phenotype possessed by select organisms to survive the harshness of winter. It is characterized by the depression of metabolic rates by as much as 99% for months, interrupted intermittently by interbout arousals lasting approximately one day. At a molecular level, expensive mechanisms are halted to conserve energy, while pro-survival genes are activated to mitigate stress. Stress granules (SGs)

and P-bodies (PBs) are quarantine sites of mRNAs that assemble upon stress induction. These cytoplasmic aggregates consist of mRNAs bound by numerous proteins, assembling upon stress exposure to control translation and to protect mRNAs from stressful elements. Given the highly stressful nature of the winter season, it was hypothesized that key regulators of SGs and PBs would be upregulated throughout hibernation. Western immunoblotting was utilized to investigate the relative abundances of these proteins during euthermia, torpor entrance, late torpor, early arousal, and interbout arousal. The results were surprising and unexpected: SG proteins were downregulated during torpor, rebounding back to baseline levels during arousal, whereas PB proteins were distinctively upregulated during arousal. The present work sheds light on an understudied facet of mammalian stress tolerance with potential relevance to cellular protection in ischemia-reperfusion injury.

A Deep Learning Approach to Identify Ganciclovir Incorporation in DNA and Understand Determinants of Cytomegalovirus Resistance

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Cytomegalovirus (CMV) is a ubiquitous herpesvirus that causes severe disease in immunocompromised individuals. Ganciclovir, a guanosine analog, is the first-line antiviral, but its effectiveness is limited by resistance mutations in the polymerase exonuclease domain. These mutations impair proofreading and alter drug incorporation dynamics, leading to drug resistance in patients. Our understanding of the mechanism is limited by the lack of an assay to measure Ganciclovir genome-wide. We present an integrated approach combining synthetic oligonucleotide design, high-throughput Oxford Nanopore sequencing, and machine learning to detect and characterize ganciclovir incorporation in DNA and uncover resistance mechanisms. To model drug incorporation, we designed oligonucleotides containing site-specific ganciclovir incorporations. Nanopore sequencing then captures the unique electrical signatures distinguishing ganciclovir from canonical nucleotides. We then use this data to train a custom deep learning model to classify incorporations with high precision. The model is applied to CMV-infected fibroblasts harboring exonuclease mutations, as well as CMV-positive patient blood samples, to reveal differences in incorporation frequency and positional bias. By linking frequency, sequence context, genomic localization, and mutation presence, we illuminate the molecular basis of ganciclovir resistance. This strategy extends beyond CMV to other antivirals and pathogens, paving the way for improved drug design and personalized interventions.

Investigating the Role of Tango2 Protein in Yeast: A Model for Rare Metabolic Disease

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TANGO2 Deficiency Disorder (TDD) is a rare metabolic disease characterized by recurrent metabolic crises, rhabdomyolysis, and arrhythmias, yet the molecular function of TANGO2 remains unresolved. To address this knowledge gap, we employ *Saccharomyces cerevisiae* as a tractable model organism to study the yeast ortholog **Tng2p (YGR127W)**. Our findings demonstrate that Tng2p localizes to peroxisomes and is essential for optimal growth on fatty acids, such as oleic acid, suggesting a role in peroxisomal β-oxidation. Genetic and biochemical assays further suggest a connection between Tng2p and **CoA metabolism**, raising the hypothesis that Tng2p functions as a “metabolite escort” for CoA and acyl-CoA species. To test this, we are performing functional complementation with human TANGO2 variants, metabolomic profiling, and genetic suppressor screening. Together, these approaches will clarify the cellular role of TANGO2 and provide mechanistic insight into TDD. This work underscores the power of humanized yeast as a model system for investigating rare diseases and may inform future therapeutic strategies.

Transcriptomic Profiling of the Plasmid Induced Cellular Burden and the Impact on Natural Product Production

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Antibiotic resistance has become increasingly commonplace in many pathogenic bacterial strains and a new method of finding antibiotics is needed to match the increasing demand. One potential method is to identify new antibiotics naturally produced by bacteria as secondary metabolites, used by bacteria to fend off other competing strains. However, bacteria tend to only express the corresponding biosynthetic gene clusters for many secondary metabolites under conditions of stress, not under ideal lab growth conditions. To increase secondary metabolite production and identify cryptic antibiotics we have induced intracellular stress, conjugating activator plasmids into a wide range of environmental bacterial strains. This has led to significant increase in the number of isolates producing antimicrobials. I have identified specific plasmid elements and media additives that have an impact on plasmid induced stress, growth rates, and secondary metabolite production. Through RNA sequencing and transcriptomic analysis, I determined the impact of plasmids on cellular stress responses and biosynthetic gene cluster expression. We also used metabolomic analysis, with LCMS, to determine levels of natural product production. The untapped biosynthetic potential of bacteria is vast, and through this work I will enable the exploration of their metabolome, allowing for the uncovering of new potentially life saving compounds.

Polymer Sciences

Development of Organic-Inorganic PN Cage-Containing Polymers as Degradable Coatings

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The development of durable materials is a key challenge in modern materials science, particularly when controlled degradation and minimization of persistent waste are considered essential for sustainability. The conception of degradable polymeric materials able to fragment at the end of their lives constitutes a promising route in sustainable materials design. In this presentation, we will highlight our recent work on a polymer system based on an activated alkyne-hydroxyl “click chemistry” between an organic monomer and a phosphorus–nitrogen inorganic cage. The results include the successful synthesis of different polymers, characterization primarily by ^{1}H and ^{31}P NMR spectroscopy, FTIR, thermogravimetric analysis and differential scanning calorimetry. Molecular weight estimation was performed using gel permeation chromatography but also DOSYNMR: this provides information on molecular diffusion, allowing an indirect estimation of molecular weight in solution. The resulting materials exhibit relatively rigid textures, likely influenced by the cage architecture.

Nanochemistry

From Eggshell to Egg yolk: Spatially Programming the Distribution of Ruthenium Nanoparticles inside a Metal–Organic Framework via Direct Incipient Wetness Impregnation

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Power-to-gas CO2 methanation can buffer variable renewables using existing gas infrastructure, potentially creating “carbon neutral batteries” without relying on traditional lithium-ion batteries. However, practical deployment requires catalysts that are efficient and durable. Metal–organic frameworks (MOFs) offer vast, ordered porosity ripe for catalysis, yet controlling where catalytically active metal nanoparticles reside inside MOFs remains largely unexplored. This work presents a direct incipient wetness impregnation (DIWI) route for embedding pre formed Ru(0) nanoparticles (~1.5 nm) into the 18 Å cages of a Zr-based MOF, MOF 808, without the need for in situ reduction of Ru(III) to Ru(0). Capillary driven infiltration during controlled solvent evaporation decouples nanoparticle synthesis from framework assembly and preserves MOF crystallinity. Framework integrity, pore occupancy, and Ru loading are established by powder X-ray diffraction, nitrogen physisorption, and inductively coupled plasma mass spectrometry, respectively. Ru speciation and location are probed by X-ray photoelectron spectroscopy, small-angle X-ray scattering and cryogenic low-dose electron microscopy, including cross sectional analysis with laser cut samples to resolve encapsulated domains. This accessible, scalable workflow turns “where the metal sits” from an accident of synthesis into a tunable design parameter that could connect internal architecture with transport and stability in methanation reactions.

Tuning Trap Depth in Er^{3+}-Doped $NaLuF_4$ Nanoparticles through Codoping Strategies

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Persistent luminescence (PersL) offers unique advantages for applications such as bioimaging and optical data storage, where the nature and distribution of charge carrier traps govern emission of light. In this work, we investigate how codoping can be used to modulate trap depth and density in β-$NaLuF_4$:Er^{3+} nanoparticles. Monovalent (Li^+, K^+) and trivalent (Fe^{3+}, La^{3+}) ions were introduced to modify the local crystal environment, and their effects were examined through structural (XRD, TEM) and optical (radioluminescence, thermoluminescence, and afterglow kinetics) characterization. Thermoluminescence measurements reveal that dopant charge and ionic radius significantly influence trap energetics: larger ions promote deeper and more thermally stable traps, while smaller aliovalent dopants enhance the population of shallower ones. These variations translate into distinct afterglow behaviours, with deeper traps leading to longer and more temperature-resistant emissions. Overall, this study demonstrates that trap depth and trap concentration can be independently tuned through rational dopant selection, providing a versatile pathway to design persistent luminescent nanomaterials with tailored optical performance.

Composition Control in Molecular Cluster-Aggregates: A Toolbox for Optical Output Tunability *via* Energy Transfer Pathways

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Composition control is an effective strategy for obtaining high-performing lanthanide (Ln) materials with tunable luminescence properties. The characteristic discrete, ladder-like energy levels of Ln^{III} make them ideal for

building systems with precise control over energy transfer processes. Recently, Ln^{III}-based molecular cluster aggregates (MCAs) have emerged as a promising platform for achieving luminescence at the nanoscale. In this work, we present a series of MCAs with icosanuclear core, $\{Ln_2Eu_2Tb_{16}\}$ (Ln = Ce, Pr, Nd, Sm, Gd, Dy, Ho, Er,Tm, and Yb), in which composition control was explored by taking advantage of its large metal core. More specifically, we investigated the effects of a third Ln^{III} doping ion on the $Tb^{III}\rightarrow Eu^{III}$ energy transfer and the ratiometric optical thermometry performance based on the Tb^{III}/Eu^{III} pair. Based on experimental data and well-known intrinsic features, such as spin−orbit coupling (SOC) strength and Ln^{III} 4*f* energy levels' structure, we discuss the possible luminescent processes present in each MCA and provide insights into qualitative trends that can be rationally correlated across the series. These findings not only deepen our understanding of the complex interplay between composition, SOC, and energy-level positions in lanthanide-based MCAs but also pave the way for the rational design of next-generation luminescent materials.

Abstracts – Poster Presentations

Organic Chemistry

Silylation of alcohol-amines for the on-demand hydrogen generation: a simple and internally catalyzed reaction

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Hydrogen-based energy is an environmentally friendly alternative to fossil fuels, but its widespread use is limited by the challenges of hydrogen production. One promising method is the on-demand generation of hydrogen through the dehydrogenative coupling of hydrosilanes and alcohol-amines. This is a single-step reaction that takes place at room temperature with no added catalysts or solvents, which represents significant advantages toward greener energy solutions compared to alternative procedures reported in the literature. The scope of the reaction was investigated using a great variety of alcohol-amines and hydrosilanes. Depending on the reactants used, more than 70 % hydrogen yield was obtained within 30 minutes of reaction. The generation of hydrogen was confirmed by gas chromatography, and the silylated products were identified by ^{13}C, ^{1}H and ^{29}Si-NMR. The main findings indicated that amine and hydroxyl functionalities in alcohol-amines are both involved in hydrogen production, being the amine groups much less reactive than the hydroxyl groups toward the hydrogen generation. It was also concluded that there is no intramolecular synergistic effect between amine and alcohol groups; however, the role of amine groups as an internal base catalyst is crucial for the performance of the reaction.

A new path towards *meta*-amino phenols

M. La Torre*, J.-P. Lumb

McGill University

The *meta*-amino phenolic pattern is at the core of 5% of the best-selling FDA-approved drugs. Despite its value, no systematic synthetic route towards this pattern has been developed. Due to the polysubstitution of the target cores (4 or more substituents) and the *meta* relationship to create, formation of the key C–N bond is challenging. Current methods such as the Buckwald-Hartwig cross-coupling or S_NAr rely on very complex halogenated precursors for selectivity, themselves difficult to source.

We report a novel method to rapidly form polysubstituted *meta*-amino phenolic cores from simple phenol and amine building blocks. To do so, we make use of *ortho*-quinone chemistry to couple phenols with nitrogen

nucleophiles and forge the C–N bond. We then convert the products to amino diazo-quinones as key precursors for downstream diversification.

This transform can become a modular tool for medicinal chemists to explore higher order substitution patterns using simple, widely available building blocks.

Development of an Efficient Methodology for the Synthesis of Fully Deprotected Oligonucleotide Dimers and Trimers

V. Petkov

McGill University

The rise in popularity of RNA therapeutics has driven a surge in research on RNA/DNA oligomers, underscoring the importance of efficient methods for the synthesis of these compounds. The recently reported resonant acoustic mixing (RAM) technique for protected oligonucleotide synthesis at gram-scale drastically reduces reaction times and solvent consumption. However, the deprotection of the resulting compounds consists of twosteps that require extreme excess of reactants and long reaction times. Our goal is to optimize the deprotection steps to match the efficiency of RAM reactions, enabling a robust, reproducible methodology for synthesizing a library of fully deprotected oligonucleotide dimers and trimers. Our starting materials consist of nucleotides with natural and modified sugars. With the RAM methodology, we couple 5'-DMT and 3'-Levulinyl protected monomers to form thiophenyl-protected phosphorothioate-linked dimers which are then subsequently coupled again to form trimers. Said dimers and trimers are then subjected to sonication and microwave irradiation to completely remove the thiophenyl and 3'-Levulinyl protecting groups in ~1.5 hours. Along with the final DMT deprotection step, all three reactions will be carried out in one pot, eliminating the need for 3 separate workups. This methodology will also be tested at gram scale, ensuring that scaleup is possible.

Streamlining Hydrogenation: Data-Driven Chemoselectivity Guide for Synthetic Chemists

K. Prystupa*, S. Newman

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Hydrogenation reactions are featured in over 40% of articles in the Journal of Medicinal Chemistry, often serving as a key step in the synthesis of bioactive molecules. Heterogeneous catalysts can effectively hydrogenate many functional groups at room temperature and low hydrogen pressure. For complex molecules, this creates challenges in chemoselectivity, typically addressed by screening inaccessible catalyst libraries. We aimed to provide chemists with a user-friendly guide for chemoselective hydrogenation, offering a more informed starting point when hydrogenation of one functional group in the presence of others is desired.

Commercial flow chemistry hydrogenation platforms like H-Cube® have emerged to minimize the safety risks of autoclave-based catalytic hydrogenation while offering better control over reaction parameters, reproducibility, heat, and mass transfer. We speculated that this would make an ideal platform for broadly assessing a range of catalysts, conditions, and substrates to design a hydrogenation user guide based on 500experiments. The reactions were conducted under progressively harsher conditions, with pressure, residence time, and temperature continuously increased. The yields of hydrogenation for each substrate and catalyst were plotted against these conditions, allowing us to tabulate the selectivity of each catalyst for different functional groups and apply our guidelines to the hydrogenation of challenging substrates.

Diaryl ether synthesis and functionalization from phenols and catechols via *ortho*-diazoquinones

V. Wu*, D.-P. Lumb

McGill University

Phenols and catechols are common functional groups of many natural products, agrochemicals and pharmaceuticals. They are also common bulk chemicals that are important building blocks of the chemical value chain. As such, they present many opportunities for methodology development in both early- and late-stage synthesis. Our group has been interested in catalytic aerobic methods for their functionalization, with the aim of developing chemoselective and atom economic tools for the preparation of polyfunctional arenes. This work outlines a deoxygenative coupling of catechols and phenols that provides 2, 4, 5-substituted diaryl ethers. The strategy hinges on a catalytic aerobic, copper-catalyzed phenol-catechol cross coupling, followed by a regioselective diazotization. The resulting *ortho*-diazoquinones are relatively uncommon synthetic intermediates but can be used as strategic intermediates from which a range of substituted arene products can be accessed. The overall transformation has the potential to be leveraged for widespread integration into the synthetic organic toolbox.

Chemistry Education

Assessing the Impact of Atropisomer Chirality on Drug Discovery and Development

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Institut National de Recherche Scientifique

Mirror-image chiral compounds can have the same primary structure but are nonetheless distinct compounds. Moreover, they can also have very different biological activities, pharmacokinetics, and toxicities profiles. Atropisomers are a class of stereoisomers that result from hindered bond rotations. Unlike classical atom-centered chiral compounds that can racemize via bond breaking, atropisomers can interconvert dynamically via simple bond rotations, with half-lives ranging from minutes to years, depending on steric and electronic factors. Thus, atropisomeric compounds are more complicated to develop.

Approximately 60% of drug discovery campaigns encounter atropisomeric properties, particularly during the lead optimization phase, where structural rigidity is often sought for optimal activity. However, the additional feature of hindered-bond chirality makes the development of atropisomers complicated because each mirror image has its own distinct properties that impacts *in vitro* and *in vivo* behaviors, including inhibition, crystallization, racemization, and ADMET profiles. Misinterpretation of results due to bond rotation can complicate development, toxicity profiles, increase costs, and pose regulatory challenges.

This poster will assess the progress made by the pharma industry in developing atropisomeric drugs since the past decade, showcasing their impact and the challenges faced in their approval and commercialization.

Environmental Chemistry

Developpement of new membranes with enhanced ammonia permeability for separation by membrane distillation

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UQAM

Ammonia is a particularly polluting compound as its fabrication accounts for ~2% of the world's CO_2 production. Furthermore, it is a well-known contaminant of wastewaters (WW), harmful to aquatic life and participating in water eutrophication. NH_3 removal in WW is usually achieved through its conversion into N_2 by nitrification and denitrification. However, considering the impact of NH_3 production, capturing it from WW in are usable form could be a way to reduce the greenhouse gas emissions associated with its production. In this study, we aim to design new additive-enhanced mixed-matrix membranes with preferential separation for ammonia in membrane distillation (MD) by studying the link between the nature and amount of additives added to the membrane and the resulting ammonia transport. Multiple NH_3-adsorbing materials were selected, namely Metal Organic Frameworks (UiO-66, UiO-66-NH_2 and UiO-66-OH) and carbon nanotubes (pristine or hydroxylated). The membranes were synthesized by phase inversion using PVDF-HFP. The results show that the addition of MOF (UiO-66) in the membrane increases ammonia recovery by up to 10 times the control value. Ongoing work will aim to compare this MOF's performance with other additives to identity the optimal material and addition ratio to enhance the ammonia separation performance of MD membranes.

Distinct Chemical Composition Profiles of Dust from Varied Sources Revealed through Targeted and Non-Targeted Analysis

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Concordia University

Urban dust acts as a reservoir for a complex mixture of organic compounds originating from traffic emissions, industrial activity, and environmental degradation. Among these, rubber- and tire-derived additives have emerged as important but undercharacterised contributors to roadway pollution. This study investigates the molecular composition of dust collected from highways, urban, and suburban sites across Montreal to assess vehicular influence among microenvironments. The objective of this work is to discover chemicals unique to each source sector. 40 samples were collected and analysed in duplicate for 80 measurements. Samples undergo solvent extraction optimised for recovering semi-volatile and polar organics, followed by high-resolution liquid chromatography–Orbitrap mass spectrometry (LC-Orbitrap-MS) analysis, allowing full-spectra high-resolution data acquisition for non-targeted screening. Non-targeted data processing reveals compositional differences among sampling locations through molecular feature extraction, alignment, and tentative annotation. Special attention is given to identifying chemical signatures indicative of tire wear and other anthropogenic inputs to urban dust. Comparative chemometric analysis will be applied to distinguish characteristic molecular signatures of roadway-derived dust. Collectively, the findings will contribute to an advanced understanding of the chemical complexity and environmental relevance of urban dust, supporting the identification of pollutant markers and their potential implications for environmental monitoring and human exposure.

Toxicological effects of drugs of abuse on aquatic organisms: bioassays with Lemna minor and Daphnia magna

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Drugs of abuse have been identified as emerging aquatic pollutants. These compounds comprise a wide range of chemical compounds, the main representatives of which are cocaine and cannabinoids. Therefore, it is essential to understand the interactions of these substances with non-target organisms. This study characterized the individual effects of cocaine (COC) and tetrahydrocannabinol (THC), when exposed to environmentally relevant concentrations, using the aquatic macrophyte Lemna minor and the microcrustacean Daphnia magna. Toxicity in L. minor was assessed at different concentrations of COC and THC for 7 days based on the measure of the number of fronds, dry weight, chlorophyll content, and levels of reactive oxygen species (ROS). Toxicity of the COC in D. magna was assessed using for 48 hours using heart rate activity in neonates. Exposure of L. minor to COC and THC induced changes in chlorophyll levels and ROS production, indicating a physiological stress response. When evaluating the effects on D. magna, heart rate remained significantly higher in exposed organisms than in the control across the tested concentrations. These findings highlight the sensitivity of both L. minor and D. magna to emerging contaminants and provide insights into the potential ecological risks of drugs of abuse in aquatic environments.

Biochemistry

Expanding Antiviral Strategies through NMR Fragment-Based Drug Discovery: The Case of SARS-CoV-2

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INRS (Institut National de la Recherche Scientifique)

NMR-based fragment drug discovery (FBDD) is a powerful method to detect weak interactions between small fragments and protein targets. Unlike high-throughput screening, which favors strong binders, NMR-FBDD can reveal shallow or hidden binding pockets inaccessible to larger molecules. It also provides early structure–activity relationship (SAR) insights while monitoring compound behavior in solution, helping to eliminate artifacts such as aggregation or poor solubility. Applying this approach to the SARS-CoV-2 non-structural protein 7 (NSP7) offers a novel direction for antiviral discovery. NSP7 is a small cofactor essential for assembling the viral polymerase complex. Targeting such a protein raises key questions: can weak NSP7 binders evolve into potent modulators of the full polymerase, and could this strategy indirectly suppress viral replication? By combining fragment-based discovery with systematic biophysical validation, NSP7 can serve as a model for understanding how weak interactions influence the function of larger replication complexes. This strategy not only broadens the scope of coronavirus drug discovery but also provides a robust framework to guide the design and optimization of new compounds through iterative medicinal chemistry strategies and advance therapeutic development against SARS-CoV-2. Moreover, this NMR-FBDD approach can be extended to other antiviral diseases.

Identifying and characterizing AML-binding aptamers for targeted delivery of RNA therapeutics

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McGill University

Acute myeloid leukemia (AML) is an aggressive blood cancer with low survival rates. New drugs are needed, potentially adopting an RNA therapeutics-based strategy, but targeted-delivery remains a major challenge. Aptamers, single-stranded nucleic acids with antibody-like affinities and specificities, are uniquely suited to overcome these challenges. For example, aptamers can be specifically developed for cancer targets and enable cell-specific uptake of drug payloads. Furthermore, aptamers have cheaper production costs and are reversible post-administration making them potentially useful as targeting-ligands. Our goal is to leverage these advantages by designing an aptamer-mediated platform for targeted delivery of RNA therapeutics to AML cells. To achieve this, we conducted an extensive literature search, identifying relevant aptamers reported to bind AML surface markers. To identify the most robust aptamers, I am characterizing each through a 2-step process: 1) measuring binding and specificity of the aptamers to a panel of AML cells via flow cytometry, then 2) quantifying affinity to isolated protein using surface plasmon resonance (SPR) and fluorescence polarization (FP). Preliminary results confirmed successful CD33 and CD117 aptamers, albeit at reduced affinities than reported. These results highlight the need for robust characterization of reported aptamers, while identifying aptamers with potential for delivering therapeutics to AML.

Contrasting ion effects in moist-solids vs. conventional dilute aqueous conditions forenzymatic cellulose depolymerization

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McGill University

The efficient depolymerization of cellulose is central to sustainable biomass valorization. Cellulase enzyme shave been used at industrial scale to degrade cellulose, typically under dilute aqueous conditions. Recent work in the Auclair lab has demonstrated that using these enzymes in moist-solid mixtures can overcome the need for substrate pre-treatment while improving yield and product selectivity. This approach, which relies on intermittent mechanical mixing, is referred to as mechanoenzymalogy. While ion-effects on enzyme activity have been studied in aqueous systems, their role in mechanoenzymatic processes remains largely unexplored. In this work, we investigate the effect of specific ions on the mechanoenzymatic depolymerization of cellulose in moist-solids. Model reactions were performed using cellulases in the presence of selected salts, and the influence of ion identity, salt-to-substrate ratio, and solid-to-liquid ratio were studied. Product formation was monitored to assess enzymatic performance.

The results show that certain salts enhance depolymerization while others strongly inhibit it. Notably, ion effects observed in mechanoenzymatic reactions did not follow the Hofmeister order typically seen in solution enzymology. This difference indicates the unique ionic environment of moist-solid mixtures, provides mechanistic insight into ion-specific influences in mechanoenzymatic cellulose processing, and highlight the potential of ion tuning in green, solvent-free biocatalysis.

Insights into mechanoenzymatic and mechanochemical depolymerization of polyhydroxybutyrate

R. N. Olegario*, J. Arciszewski, M. S. Chi, K. Auclair

McGill University

Plastic waste is one of the biggest environmental concerns facing today's world, with 359 million tons of plastic generated in 2024 and only a small fraction thereof being recycled. Biopolymers such as polyhydroxybutyrate (PHB) offer a more sustainable approach to consumer plastics, but its biodegradability is very slow and limited by soil conditions. The depolymerization of PHB would enable the breakdown of PHB into its constituent monomers for closed-loop recycling or for use as a chemical feedstock. To achieve greener depolymerization, mechanochemistry – which almost entirely eschews the use of bulk solvent – enables potent reactivity while potentially mitigating the need for substrate pretreatment. The combination of mechanochemistry with enzymatic catalysis, dubbed mechanoenzymology, places enzymes in a mechanically mixed environment with only tiny amounts of water, minimizing water waste. This environment has also been demonstrated to afford greater yields and selectivity for many enzymes, as well as unique mechanistic effects. This presentation will summarize our progress towards the depolymerization of PHB using both mechanochemical and mechanoenzymatic approaches.

Evaluation of the importance of SUMO interaction motifs (SIMs) in the design of novel synthetic SUMO E3 ligases and identification of promising candidates for biotechnological applications

H.-W. Petit-Frere

UQAM

SUMOylation is a critical post-translational modification that regulates diverse cellular functions, including protein stability and interactions. It occurs via an enzymatic cascade involving E1, E2, and E3 ligase enzymes, which stimulate SUMO transfer to lysine residues of target proteins. All known E3 ligases possess short sequences called SUMO-interacting motifs (SIMs) that optimally position SUMO for transfer. However, the precise role of SIMs in SUMO E3 ligase activity remains poorly explored. The objective of this project is to investigate the importance of SIMs in SUMO E3 ligase activity, including ZNF451, an atypical SUMO E3 ligase with two SIMs essential for its function. By replacing these SIMs with optimized sequences, it is hoped to design novel synthetic SUMO E3 ligases capable of promoting the stabilization of target proteins for therapeutic and biotechnological purposes. Thus, this project could lead to the development of "SUMOTACs", a concept parallel to PROTACs, but intended to promote the stabilization of proteins via SUMOylation, instead of targeting them for degradation.

The Role of Metal Ions in DNA-Guided Assembly of Carbonic Anhydrase II Active Site

V. Zhang*, F. Zhao, H. Sleiman

McGill University

Enzymes are versatile biomolecules that perform diverse functions, and are workhorses in green chemistry and industries for sustainable drug synthesis. While studies of entire enzymes face challenges of cost and sensitivity, application of synthetic protein mimics is a more affordable approach to explore of unstudied sequence space and modifications.

Carbonic anhydrases (CA) are Zn metalloenzymes that are well characterized for their high efficiency and capability for carbon capture. Here we report the potential modifications and metal ion substitutions of CA II

using DNA-guided assembly - using DNA as scaffold to assemble synthetic peptide strands into new artificial proteins - to replicate Carbonic anhydrases (CA) II active site with increased stability. A structural mimic of CAII was created by covalently linking three a-helices bearing the Zn-active site residues to three DNA strands, and hybridizing with a trimeric template to stabilize the assembly. The Zn2+ coordinated mimic was characterized by CD and exhibit esterase activity. Structural and kinetic analyses of Co2+, Cu2+, and Ni2+ substituted mimics will be described. This work validates the application of active site mimetics as tools for enzymatic studies and demonstrates the potential of new catalysis in carbonic anhydrase II by metal ion substitution.

Targeting Cryptic Pockets: A Fragment-Based Screening Approach

S. Rezaeian*, S. R. LaPlante

INRS

VP35, a key Ebola virus protein, plays a critical role in immune evasion and viral replication, making it an attractive target for antiviral drug discovery. Recent studies have identified a cryptic pocket within VP35 1, which could serve as a potential binding site for small-molecule inhibitors. However, targeting cryptic pockets requires advanced screening and validation techniques due to their transient nature. Our research team applied a combination of biophysical methods to screen a fragment library and identify initial hit compounds targeting this cryptic pocket. Using our novel ligand-detection approach which includes the NMR experiments T2-CPMG, Differential Line Broadening (DLB), Differential Line Broadening and Shifting (DLBS) and STD 2. To complement these experimental findings, molecular docking was employed to help predict the relationship between the dynamic flexibility of VP35 and the formation of the fragment binding pocket. Together, the experimental NMR screen and the molecular dynamics calculations will allow us to predict the existence of cryptic pockets for a wide variety of protein targets along with discovering fragment seeds for future drugs.

Inorganic Chemistry

Effect of tetraphenylborate (BPh_4^-) on the catalytic and biological activity of organoruthenium complexes

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Our research program aims at creating metal-based therapeutics that could potentially overcome problems associated with existing chemotherapies. Ruthenium complexes hold promise as alternatives to the platinum drugs. Known to display their anticancer activity via various modes of action, some ruthenium-based complexes were recently reported to act as intracellular catalysts, able to selectively kill cancer cells by promoting the transfer hydrogenation of NAD^+ to NADH. This catalytic transformation has emerged as a potential way to irradicate cancer cells, by modulating the cells' redox status. As cancer cells are more sensitive than healthy cells to small changes in their NAD^+/NADH ratio, Ru-based complexes could lead to the development of a selective treatment. Previous studies have shown that introducing a tetraphenylborate anion (BPh_4^-) within the structure of organoruthenium complexes enhances their activity against certain cancers, notably against triple-negative breast cancer (TNBC). Based on the above-described concept and intrigued by the role of the BPh_4^- on catalytic and anticancer activities of organoruthenium complexes, we are investigating the impact of incorporating BPh_4^- into catalysts known for efficiently promoting the transfer hydrogenation of NAD^+ to NADH. In this presentation, we will share our latest findings and our future plans regarding this developing project.

Hydrosilane-mediated activation of B-O bonds for sustainable Boron recycling in cross-coupling reactions

D. Girish*, F. Fontaine

Laval University

Organoboron compounds are versatile reagents in modern organic synthesis due to their distinctive electronic properties, structural adaptability, and utility in key bond-forming reactions, such as the Miyaura-Suzuki and Chan-Lam couplings. Despite significant advances in B-X (X = B, C, Si, Cl, Br, I) bond chemistry, the activation of the robust B-O bond remains largely unexplored. The exceptional stability of B-O-containing boronate species often renders them synthetically inert, leading to their accumulation as terminal byproducts.

In this work, we intend to explore different strategies to perform B-O bond activation employing readily available and non-toxic hydrosilanes. Preliminary DFT studies support the thermodynamic feasibility of the activation process and regeneration of a synthetically valuable boron intermediate. These regenerated species will later be utilized in the Miyaura-Suzuki Coupling reactions to demonstrate their reactivity and synthetic competence. Hence, we seek to establish a catalytic process for the recycling of Boron in chemical transformations, transforming otherwise discarded boron products into reusable reagents and contributing to sustainable, atom-economical methodologies in synthetic chemistry.

Innovative N,O-Bidentate Ligands for Enhancing the Photoactivity of First-Row Transition Metal Complexes

C. Gros[1]*, A. Saha[1], M. Cibian[2], G. S. Hanan[1]

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Bidentate N, O ligands are promising for the development of photoactive first-row transition metal complexes. Among them, amidines *N*-oxide (AMOX) derivatives *(Figure 1*) are synthesized by *N*-oxidation of parent amidines using *m*-CPBA. Their corresponding complexes, such as Co(AMOX-Ph-CN)$_3$ (*Figure 1*), exhibit interesting photophysical properties for potential applications in catalysis and artificial photosynthesis. This study will focus on optimizing the synthesis of these ligands and their complexes, while providing detailed characterization through NMR and UV-vis spectroscopy, and X-ray diffraction analysis. Additionally, the potential to polymerize photoactive materials, incorporating first-row metal complexes, will be explored, targeting antenna effects or new magnetic properties for future applications.

Development of carbene-supported half-sandwich Rh complexes for H2 storage applications

C. McDonald*, S. Pal

Brandon University

Depletion of fossil fuels and reductions in climate-impacting emissions necessitate clean fuels to meet future energy demands sustainably. Hydrogen (H_2) is a leading alternative to fossil fuels, offering high energy density and clean combustion. Current bottlenecks to widespread H2 incorporation include storage limitations and safety concerns – for viability, production and storage need to occur at near atmospheric pressures. This can be achieved through the incorporation of light organic hydrogen carriers (LOHCs) as H2 surrogates. To be leveraged, LOHCs require a bi-directional catalyst for reversible H2 production and storage at atmospheric pressures. ‘Half-sandwich’ rhodium complexes with 1,2,3,4,5-Pentamethylcyclopentadiene (Cp*) ligands are a popular class of catalysts used in (de)hydrogenation reactions. By fine-tuning ancillary ligands, catalytic efficiency can be enhanced. Comparing di-imidazolium methane (dimm) Cp*Rh complexes recently developed

in our lab to the previously reported 2,2-bipyridine (bpy) analogues, we find that dimm renders the Rh center substantially more electron rich, implying more efficient catalysis. Protocols for high-throughput ligand synthesis, preparation of Cp*Rh complexes and computational insights into catalytic mechanisms will be discussed.

Versatility of PN Ligands in Photocatalysis: Tailored Ni(II) and Ru Complexes for H2 Generation and CO2 Conversion

E. Mohamad*, D. Richeson

University of Ottawa

The pursuit of sustainable green energy sources has intensified the search for efficient, earth-abundant catalysts. We report significant advancements in photocatalytic systems utilizing versatile PN-coordinating ligands with nickel and ruthenium complexes. This work addresses two important challenges: hydrogen production and CO_2 conversion. Well-defined, air-stable nickel (II) complexes catalyzed photocatalytic acceptorless alcohol dehydrogenation (AAD) for hydrogen production. This system operates effectively at room temperature under visible light irradiation, enabling selective hydrogen generation from various aliphatic alcohols. The introduction of dimethylethanolamine (DMEA) as a novel electron donor significantly enhances catalyst performance. Concurrently, we have developed new visible-light CO_2-reducing photocatalysts based on ruthenium complexes supported by PN ligands. We explored the versatility of both catalyst systems by varying ligands, electron donors, and solvents. Mechanistic studies, supported by computational analysis, reveal the crucial role of the flexible PN ligands in facilitating the catalytic cycles. This work addresses challenges in sustainable hydrogen production and CO_2 utilization and showcases the versatility of PN ligands in tailoring transition metal complexes for traditional catalysis and photoredox chemistry.

Homoleptic cobalt(III) bisguanidylpyridine complexes for photocatalytic and photoredox processes

I. Oubaha[1]*, A. K. Pal[2], G. S. Hanan[3]

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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 (E1/2(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}MCstate. Herein we present a new photoredox catalyst for the regioselective mono trifluoromethylation of polyarene but also for the photosynthesis of H_2.

Metal–Organic Frameworks for Direct Air Capture of Carbon Dioxide

J. Singh[1]*, A. Howarth[1], C. Copeman[1], P. De Luna

[1]Concordia University, [2]Deep Sky Inc,

Direct air capture (DAC) is a promising technology that can help remove CO_2 from the air, but it relies on effective sorbents. Metal–organic frameworks (MOFs) have gained attention as potential sorbents due to their high surface area, tunable chemistry, and porosity. To accelerate the discovery of MOFs for DAC, Meta AI

developed the *Open DAC 2023 dataset*, which provides large-scale DFT adsorption energies for CO_2 and H_2O adsorption in pristine and defective MOFs. More recently, the *GoldDAC dataset* was introduced, focusing on a smaller curated set of MOFs screened entirely with DFT to yield more accurate binding energies. While the *Open DAC 2023 dataset* emphasizes scale and diversity, the *GoldDAC dataset* emphasizes accuracy, leading to differences in the MOFs predicted to be most promising for DAC. In this work, the top 10 MOFs recommended for DAC from the *Open DAC 2023 dataset* and 3 of the 12 top-ranked MOFs from the *GoldDAC dataset* were synthesized and tested for CO_2 and H_2O adsorption, alongside several well-known MOFs as benchmarks. The selected MOFs were characterized using powder X-ray diffraction, thermogravimetric analysis, N_2 and H_2O adsorption-desorption, and tested for CO_2 uptake from 0 to 1 atm, focusing on 400 ppm CO_2.

Sustainable Production of a Zirconium Metal–Organic Framework Through Optimization of Washing Steps

L. Thomas*, C. Copeman, A. J. Howarth

Concordia University

Zirconium-based metal–organic frameworks (MOFs) are among the most thermally and chemically stable classes of MOFs. Due to their versatility and high stability, they have been studied for a diverse array of applications, including catalysis, gas storage, wastewater remediation, and more. The current synthetic process for the vast majority of zirconium MOFs are time-intensive and require large volumes of N,N-dimethylformamide (DMF) as a washing solvent, which poses environmental concerns. This study examines the effects of a greener washing method, as well as reduced solvent washing contact time, and the effects of systematic changes on the final physical properties of a zirconium-based MOF. Structural characterization is primarily performed using powder X-ray diffraction (PXRD) and nitrogen gas adsorption analysis. Replacing the DMF washing solvent with water, while also reducing both the intervals between washes and the number of washes, increased synthetic throughput without compromising the high surface area and structural integrity of the MOF, demonstrating an effective, sustainable, and efficient preparation method.

Analytical Chemistry

Feasibility of Protein Detection from a Single-Cell via Capillary Zone Electrophoresis Laser-Induced Fluorescence

C. Leung*, C. Skinner

Concordia University

Single-cell analysis is pivotal for understanding cell-to-cell variations in gene expression, protein levels, and other parameters that bulk averaging may overlook. This study uses known concentrations of HeLa cells as the model for human cells. The cells were concentrated, lysed by denaturation, and labeled with a primary-amine specific dye, FQ atto-tag. The lysate was separated by capillary zone electrophoresis and the fluorescent signal measurements were correlated with calculated cell equivalents. Preliminary results demonstrated successful disruption and labeling, with protein content measured at 0.1 cell equivalent on-column. To further validate the approach, fresh cells were concentrated to a higher level, processed, and analyzed, revealing additional peaks in the electropherogram at a final concentration of 0.5 cell equivalent on-column. These findings suggest that single-cell detection is achievable with optimized sample preparation and further sensitivity enhancements are readily achievable.

Computational Chemistry

Virtual Chemist: computer-aided design in asymmetric catalysis

J. Genzling*, S. Pinus, Z. Luo, B. Weiser, Y. Wong, N. Moitessier

McGill University

The field of asymmetric catalysis has revolutionized organic synthesis over the past 50 years by enabling new reactions, accelerating others, and promoting the synthesis of a single stereoisomer as the main product. However, developing new chiral catalysts remains a significant challenge, often requiring a lengthy, laborious process.

To address these challenges, we developed **Virtual Chemist (VC)**, a computational platform integrating physics-based methods to predict stereoselectivity. While VC has successfully reproduced over 350 stereoselectivities across multiple reaction classes, its accuracy remains insufficient for ranking catalysts. This poster presents anew approach to enhance VC by refining its molecular mechanics scoring force field using machine learning. By retraining selected force field terms on a large dataset of VC-transition state energies and geometries, we aim to introduce a "**transition state–aware" flavor to the energy scoring**. This data-driven refinement improves both accuracy and transferability across reaction classes, enabling more reliable catalyst ranking. This will be demonstrated in an asymmetric organocatalyzed Diels-Alder reaction, where the reaction mechanism was studied in greater detail. In particular, our group was able to show that the pKa of various catalysts could be linked to the catalytic activity and hence build a pKa predictor based on Graph Neural Network.

Advancing Aptamer Design Through Machine Learning Methods

A. Najera

McGill University

Nucleic acid-based therapies have transformed medicine, as shown by the success of mRNA vaccines and FDA-approved therapeutic oligonucleotides. Yet, these therapies often accumulate in the liver and kidneys, limiting their use for other diseases. Aptamers are single-stranded oligonucleotides that bind proteins with high affinity and offer a novel strategy for targeted delivery. They are inexpensive and structurally versatile, but their exploration is usually limited to the four natural nucleobases. Selection methods such as SELEX also face constraints in scalability, speed, and chemical diversity. We propose a computational–experimental platform to accelerate the discovery of chemically modified aptamers for targeted delivery of nucleic acid-based therapies. The approach integrates machine learning models with experimental validation. Models incorporate chemical properties of modified nucleotides and molecular descriptors of protein targets to predict affinity and specificity across millions of sequences. Top candidates will be synthesized and tested in biophysical and cellular assays, creating a feedback loop that progressively improves predictive accuracy. This interdisciplinary strategy will enable faster development cycles, expand the accessible chemical space, and identify novel molecular architectures. The platform aims to provide modular, adaptable tools for cell-specific delivery of aptamer-based therapeutics, addressing a critical challenge in the pharmaceutical industry and advancing personalized medicine.

Predicting the folding of single-stranded DNA aptamers using a machine-learned coarse-grained force field

M. E. Toloue Sadegh Azadi*, L. Simine

McGill University

Aptamers are single-stranded DNA and RNA molecules that can specifically bind to a wide range of biological targets. DNA aptamer structures depend on solution conditions and can be disrupted by pH, temperature, and ionic strength, making their modeling challenging. We re-purpose a machine-learned coarse-grained (CG) forcefield, previously proposed by Clementi group for peptides, training it on atomistic aptamer simulations to enable transferability to unseen sequences for tertiary structure prediction. The model learns the potential of mean force (PMF) through a force-matching scheme, minimizing the difference between predicted and atomistic forces. Four DNA aptamer sequences with known structures were each simulated for 25 nanoseconds, and the resulting trajectories were used to train the model. The model successfully converged at a minimum loss of 119, demonstrating its potential to learn CG interactions. To ensure physical fidelity, we incorporate a physics-informed prior energy model including bonded, angular, dihedral, and non-bonded terms. This scheme constrains unphysical motions while maintaining flexibility for folding pathways. To track the folding process, we construct contact maps for each simulation and assess contact stability. We examine DNA aptamer folding and assess the impact of the CG force field with physics-informed priors, additional sequences, and more MD simulation frames.

SO(3) Equivariant Embeddings for Transition State Prediction

S. Zhang*, R. Khaliullin

McGill University

An artificial neural network is equivariant to a symmetry operation if the order of performing the symmetry operation on the data and the neural network on the data commute. SO(3) is the special orthogonal group of continuous 3d rotations, which we expect chemical species to obey. Traditional neural networks for chemistry are either non-equvariant, or invariant, a special and restricted case of equivariance. Recent works have used equivariant embeddings for chemistry, though as part of a complex graph-neural-network. We use explicitly SO(3) equivariant neurons and activation functions to learn on point-cloud chemical data, and learn embeddings that allow predictions of transition state structures and energies. We show that rotational equivariance alone is competitive with rotational equivariance in combination with graph equivariance for transition state tasks.

Molecular Biology

Identification of freeze-responsive microRNAs in vertebrate hearts: Novel insights into cardiovascular disease

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Carleton University

A major barrier in both cryopreservation and myocardial infarction is preventing cell damage caused by disrupted energy homeostasis and the proliferation of reactive oxygen species (ROS) during reperfusion. The freeze-tolerant wood frog (*Lithobates sylvaticus*) provides a compelling natural model for overcoming these challenges, as it can survive weeks of whole-body freezing accompanied by global ischemia, anoxia, and oxidative stress. Survival is achieved through metabolic rate depression, reprioritization of energy use,

accumulation of cryoprotectants, and anticipatory antioxidant defenses that mitigate ROS damage upon thaw. To uncover post-transcriptional regulatory mechanisms underlying these adaptations, small RNA sequencing was performed on active and frozen wood frog hearts, followed by GO and KEGG pathway analyses. Among 23detected miRNAs, three were significantly altered following freezing (miR-9983-3p, miR-24-3p, miR-1973). miR-24-3p, which interacts with key cardiac ischemia regulators (HMGB1, ETS1, EGR1), was upregulated, suggesting a potential cardioprotective role during freezing and thaw. In contrast, miR-1973 was downregulated, potentially contributing to transcriptional repression and energy conservation. Overall, the data suggest that differential miRNA regulation promotes cardioprotection and facilitates metabolic rate depression during whole-body freezing, offering insights relevant to improving cryopreservation and ischemic injury therapies.

Treating Infections by Inhibiting Growth Under Infection-Relevant Conditions

S. Diaconescu-Grabari[1]*, J. Pierscianowski[1], A. McAlpine[1], C. B. Lan[1], A. B. Abdelaal[1], A. Pierret[1], I. Roe[2], A. Lupien[2]

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The number of antibiotic-resistant infections is rapidly increasing. The development of new strategies to combat them is essential, and a focus is placed on treatments that slow resistance development. One strategy used in the Auclair Lab to combat AMR is to create novel antibacterials active only under infection-relevant conditions. Specifically, we are interested in intracellular bacteria, such as *Salmonella enterica* ser. Typhimurium (STm), *Mycobacterium tuberculosis*, and *Pseudomonas aeruginosa*, which can proliferate inside macrophages, making them difficult to eliminate and treat. Macrophages engulf bacteria, providing harsh conditions meant to kill them. However, these pathogens take advantage of these conditions and thrive in macrophages.

We seek molecules that selectively prevent the proliferation of intracellular bacteria, without affecting extracellular ones, as we expect reduced resistance selection under these limited conditions. To do this, compounds designed and synthesized in our lab were tested for their ability to inhibit the growth of STm in a variety of media, modelling both extracellular and intracellular environments. Molecules that showed activity only in the latter were tested for their ability to reduce the proliferation of STm in macrophages. Two compounds were tested *in vivo* and found to significantly decrease the STm burden in a colitis mouse model.

Size-Based Flow Cytometry Sorting for Distinguishing Quiescent and Non-Quiescent Yeast Subpopulations

D. Gokbayrak*, C. Brett

Concordia University

Baker’s yeast (Saccharomyces cerevisiae) is a powerful model for studying replicative aging, defined by the number of daughter cells produced before senescence, and chronological aging, reflecting the survival of non-dividing, stationary-phase cells. Within yeast populations, quiescent and non-quiescent (mother, and daughter) cells exhibit distinct physiological states that reveal conserved mechanisms of cellular maintenance, stress adaptation, and longevity relevant to human aging. Vacuolar function is central to these processes, as it regulates ion and pH balance, mediates the clearance of damaged proteins and organelles and supports lipid and amino acid homeostasis. Preservation of vacuolar integrity enhances stress resistance and lifespan across all three subpopulations. Conventional centrifugation-based methods for separating quiescent and non-quiescent cells are time-consuming, reagent-intensive, and can disrupt yeast morphology and vacuolar

integrity. To address these limitations, we developed a flow cytometry–based sorting strategy that discriminates yeast cells by size and complexity into quiescent, daughter, and mother populations. This approach enables rapid, reproducible, and morphology-preserving isolation of subpopulations. It provides a scalable platform for molecular, metabolic, and phenotypic analyses of yeast aging and offers a broadly applicable framework for exploring conserved pathways of cellular aging in eukaryotic systems.

Spatiotemporal regulation of Ect2, a proto-oncogene that is critical for cytokinesis

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Concordia University

Cytokinesis, the final stage of the cell cycle, ensures proper cell division by forming a RhoA-dependent actomyosin contractile ring. This process must be tightly coordinated with chromosome segregation to prevent aneuploidy and disease. Ect2, a guanine nucleotide exchange factor, activates RhoA to drive ring assembly, but its regulation remains unclear. Our research reveals that active Ran, associated with segregating chromosomes, creates an enriched zone of importins that modulate ring assembly. Importins typically bind to nuclear localization signals (NLSs) in proteins which are released by active Ran. Ect2 contains a predicted NLS within its C-terminus, and we determined if importin-binding regulates its function. We show that GST:Importin-βbinds to fragments of Ect2 containing the NLS from HeLa cell lysates, and point mutations disrupt binding. RNAi-resistant mScarlet-tagged Ect2 NLS mutants in cells depleted of endogenous Ect2 failed to localize to the equatorial membrane and caused cytokinesis failure. The NLS also harbors a consensus Cdk1 phosphorylation site. Since NLS residues are basic, we hypothesized that phosphorylation could block importin-binding. Indeed, a phosphomimetic mutant abolished Importin-β binding and membrane localization. Since Cdk1 activity declines during mitotic exit, this may serve as a timing mechanism for Ect2 recruitment. Therefore, Importin-β regulatesEct2 localization and function during division.

Polymer Sciences

Spatiotemporally controlled formation of DOPA-based biomaterials

L. (. Huang

McGill University

DOPA (3,4-dihydroxyphenylalanine) exhibited self-healing, rapid curing adhesion properties in marine organisms. In vitro, the synthesis of DOPA is constrained by challenges in controlling its redox chemistry. A styrosinase-mediated oxidation of tyrosine often proceeds beyond DOPA to DOPA-quinone, suppressing metal coordination and crosslinking. Mussels naturally overcome this by compartmentalizing DOPA-rich proteins and metal ions within secretory vesicles, where microenvironments regulate crosslinking with high precision. Coacervates resemble vesicles in their ability to compartmentalize molecules, they form as dense liquid droplets of polymers or peptides through spontaneous liquid–liquid phase separation. They can be engineered to interact with metal ions and biomolecules selectively. Inspired by this strategy, we aim to develop coacervates with a charged semi-permeable lipid shell, creating a compartmentalized environment for precise spatiotemporal control of DOPA production. Tyrosinase is encapsulated before lipid assembly, while the charged membrane admits small peptides but excludes metal ions due to electrostatic repulsion. Inside, tyrosinase converts tyrosine to DOPA, which subsequently diffuses into the bulk to complex with metal ions, forming extended crosslinked networks. This two-stage process prevents further oxidation and enables tunable DOPA–metal assemblies. Our approach establishes spatiotemporal regulation of DOPA chemistry and provides a versatile platform for biomedical adhesives, hydrogels, and self-healing coatings.

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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 28th 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 28e édition du CBGRC.

Le Comité Organisateur