CONCORDIA
UNIVERSITY

24th ANNUAL CONFERENCE

NOVEMBER 19th, 2021

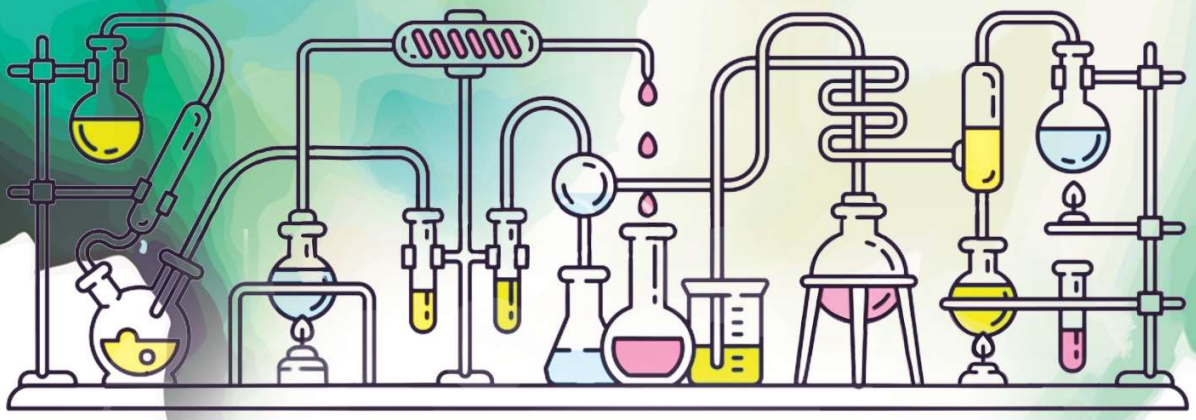
ONLINE EVENT

KEYNOTE SPEAKERS

Dr. Todd Hyster
Dr. Geoffrey Ozin

OCTOBER 30th

REGISTRATION DEADLINE



CBGRC

Chemistry and Biochemistry Graduate Research Conference

www.concordia.ca/CBGRC
INFORMATION

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WELCOME NOTE // LETTRE DE BIENVENUE

Dear friends and colleagues,

We are very excited to welcome everyone to the 24th annual Chemistry and Biochemistry Graduate Research Conference. The goal of the CBGRC has always been to gather graduate students, professors and industry representatives in order to have them share their knowledge and research in a welcoming environment. This year we find ourselves in a transitional period where the scientific community has had to learn how to thrive under the many restriction of the pandemic while slowly finding ourselves able to re-expand our practices once again. It is easy to see globally this experience has allowed the scientific community to expand its connective network as one of the greatest results from these past two years has been to the international collaboration seen between scientists all across the world. The CBGRC celebrates the achievements we've made and aims to showcase them here with presenters from around the world. Although the conference is once again online, we hope to provide an amazing at-home experience and to inspire your research to new heights. We would like to thank everyone for your help in making the CBGRC a continued success, and we look forward to listening to your presentations and hopefully see you all in person next year.

The CBGRC Organizing Committee

Cher(e)s ami(e)s et collègues,

Nous sommes très heureux d'accueillir tout le monde à la 24e conférence annuelle de recherche des diplômés en chimie et biochimie. L'objectif du CRCSCB a toujours été de rassembler des étudiants diplômés, des professeurs et des représentants de l'industrie afin de leur faire partager leurs connaissances et leurs recherches dans un environnement accueillant. Cette année, nous nous trouvons dans une période de transition où la communauté scientifique a dû apprendre à prospérer sous les nombreuses restrictions de la pandémie tout en nous trouvant lentement en mesure de ré-établir nos pratiques une fois de plus. Il est facile de voir à l'échelle mondiale que cette expérience a permis à la communauté scientifique d'étendre son réseau de recherche car l'un des plus grands résultats de ces deux dernières années a été la collaboration internationale observée entre les scientifiques du monde entier. Le CBGRC célèbre les réalisations que nous avons accomplies et vise à les présenter ici avec des représentants du monde entier. Bien que la conférence soit à nouveau en ligne, nous espérons offrir une expérience à domicile incroyable et inspirer vos recherches vers de nouveaux sommets. Nous tenons à remercier tout le monde pour votre aide à faire du CBGRC un succès continu, et nous sommes impatients d'écouter vos présentations et espérons vous voir tous en personne l'année prochaine.

Le Comité Organisateur de la CRCSCB

MORNING KEYNOTE SPEAKER — DR. TODD HYSTER // 10:00 AM EST

ABOUT DR. HYSTER

Todd is a native of Apple Valley, Minnesota, and did his undergraduate studies at the University of Minnesota. In 2008 he joined Tomislav Rovis' group at Colorado State University for his graduate studies to develop Rhodium-catalyzed C–H activation reactions. During his Ph.D., Todd did an internship with Thomas Ward at the University of Basel where he prepared an artificial metalloenzyme for an asymmetric C–H activation reaction. After graduating, he joined the group of Frances Arnold at Caltech as an NIH Postdoctoral Fellow. In the Arnold group, Todd evolved P450s to catalyze nitrene transfer reactions. In 2015 he started his independent career at Princeton University and in 2021 moved to Cornell University, where he is currently an Associate Professor of Chemistry and Chemical Biology. Todd's group has developed photochemical strategies to expand the synthetic utility of common enzymes, enabling them to address long-standing selectivity challenges in the chemical synthesis literature.

ABSTRACT: DEVELOPING BIOCATALYSTS FOR THE 21ST CENTURY

Enzymes are exquisite catalysts for chemical synthesis, capable of providing unparalleled levels of chemo-, regio-, diastereo- and enantioselectivity. Unfortunately, biocatalysts are often limited to the reactivity patterns found in nature. In this talk, I will share my groups efforts to use light to expand the reactivity profile of enzymes. In our studies, we have exploited the photoexcited state of common biological cofactors, such as NADH and FMN to facilitate electron transfer to substrates bound within enzyme active sites. In other studies, we found that enzymes will electronically activate bound substrates for electron transfer. In the presence of common photoredox catalysts, this activation can be used to direct radical formation to enzyme active sites. Using these approaches, we are able to develop biocatalysts to solve long-standing selectivity challenges in chemical synthesis.

AFTERNOON KEYNOTE SPEAKER – DR. GEOFFREY OZIN // 3:30 PM EST

ABOUT DR. OZIN

Geoffrey A. Ozin is a Distinguished University Professor at the University of Toronto and Tier 1 Government of Canada Research Chair in Materials Chemistry and Nanochemistry. He currently spearheads the Solar Fuels Group at the University of Toronto. He has held positions as Honorary Professor at The Royal Institution of Great Britain and University College London, External Adviser for the London Centre for Nanotechnology, Alexander von Humboldt Senior Scientist at the Max Planck Institute for Surface and Colloid Science and the Center for Functional Nanostructures at the Karlsruhe Institute of Technology, and Global Chair at Bath University. He is the author of four books: Nanochemistry: A Chemical Approach to Nanomaterials (RSC 2006), Concepts of Nanochemistry (Wiley-VCH 2009), The Story of CO2: Big Ideas for a Small Molecule (UTP 2020), and Energy Materials Discovery Enables a Sustainable Future (RSC 2021), and recipient of many National and International Awards, recent ones include World Cultural Council Albert Einstein science Prize, World Technology Network Energy Prize, Royal Society of Chemistry Centenary Award. He lives with his wife in Toronto, Canada.

ABSTRACT: SAVE THE WORLD-SHINING LIGHT ON CO_2

Energy makes the world go round, we have plenty of it, and it is mainly fossil sourced. In 2020 we used 23,000 TWh, that's the good news, the bad news is that the 40 billion tons of CO_2 emitted into our atmosphere from its production, distribution, and use is now posing an existential threat to life on earth, and it is getting worse. The latest IPCC report flags 'code red' for humanity, unless we act fast. The solution is simple on paper but complex in practice; transition from fossil to renewable forms of energy using known technologies that work, can be scaled, implemented over a decade or so, and go global. While not a panacea, one approach to help ameliorate climate change, is to decarbonize the fossil powered and fossil sourced chemical and petrochemical industries using CO_2 as the feedstock. Manufacturers of hundreds of millions of tons of chemicals and fuels, these industries would not exist without catalysts; more than 90% are heterogeneous, their production represents a $8.5 billion per year market, and the gross annual sales of chemicals synthesized by catalysis is $3 trillion. Currently, most of these catalytic processes are driven by fossil heat and are responsible for about 2.3 billion tons of CO2 emissions, about 5.8% of global greenhouse gas emissions. Syngas, a fossil derived mixture of CO and H_2, is a primary feedstock for hundreds of thousands of commodity chemicals and many transportation fuels. Commercially available technology exists, for making syngas from CO_2 and H_2O feedstocks, mainly driven by heat, thermochemically. Why not power them with light, photochemically? In this presentation I will look what is around the bend in this emerging field, especially the most recent focus on how to engineer high photon efficiency photocatalysts and photoreactors to produce solar syngas, a sustainable feedstock for solar chemicals and fuels.

ROOM LINKS OVERVIEW AND CONFERENCE GUIDELINES

ROOM	LINK
1	https://concordia-ca.zoom.us/my/cbgrc1
2	https://concordia-ca.zoom.us/my/cbgrc2
3	https://concordia-ca.zoom.us/my/cbgrc3
4	https://concordia-ca.zoom.us/my/cbgrc4
5	https://concordia-ca.zoom.us/my/cbgrc5

CONFERENCE GUIDELINES:

- Please enter your Zoom session 5 minutes before the session begins.
- All presenters will be given screen sharing capabilities to present their visual aid during their presentation.
- Have a good quality microphone and station yourself in a room without background noises or echoes.
- Make sure your microphone is muted when you are listening to the presentations of your peers.
- While a webcam is strongly recommended for improved engagement with your audience, it is not mandatory.
- Ensure your name on Zoom and in your presentation is the same as the one used to register on the conferencereg.com/cbgrc website.
- ***Especially for shotgun presentations,*** include contact information in the form of an email address or QR code at the end of your presentation, in case someone in your audience would like to contact you for potential questions or discussions.
- Recording oral presentations and shotgun talks is strictly prohibited.
- All times are in EST.
- If you need help with anything, email cbgrc.concordia@gmail.com

SCHEDULE OVERVIEW

TIME (EST)	EVENT	LINKS
07:30 - 8:00	Welcome Announcement	CBGRC ROOM 1
08:00 - 09:45	Talk Session A	CBGRC ROOM 1 PHYSICAL CHEMISTRY CBGRC ROOM 2 BIOCHEMISTRY CBGRC ROOM 3 ANALYTICAL CHEMISTRY CBGRC ROOM 4 MOLECULAR BIOLOGY CBGRC ROOM 5 INORGANIC CHEMISTRY
10:00 – 11:00	Keynote Speaker – Dr. Todd Hyster	CBGRC ROOM 1
11:15 – 12:45	Talk Session B	CBGRC ROOM 1 ENVIRONMENTAL & ANALYTICAL CHEMISTRY CBGRC ROOM 2 BIOCHEMISTRY & MOLECULAR BIOLOGY CBGRC ROOM 3 ORGANIC CHEMISTRY CBGRC ROOM 4 COMPUTATIONAL CHEMISTRY CBGRC ROOM 5 INORGANIC CHEMISTRY
12:45 - 13:30	Lunch	
13:30 – 15:15	Talk Session C	CBGRC ROOM 1 PHYSICAL CHEMISTRY CBGRC ROOM 2 BIOCHEMISTRY CBGRC ROOM 3 ORGANIC CHEMISTRY CBGRC ROOM 4 BIOCHEMISTRY CBGRC ROOM 5 NANOCHEMISTRY
15:30 – 16:30	Keynote Speaker – Dr. Geoffrey Ozin	CBGRC ROOM 1
16:45 – 18:00	Shotgun Presentations	CBGRC ROOM 1 INORGANIC & ORGANIC CHEMISTRY CBGRC ROOM 2 MOLECULAR BIOLOGY CBGRC ROOM 3 BIOCHEMISTRY CBGRC ROOM 4 ENVIRONMENTAL, ANALYTICAL, NANO- & PHYSICAL CHEMISTRY
18:00 - 19:30	Break	CBGRC ROOM 1
19:30	Award Announcements	CBGRC ROOM 1

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

PHYSICAL CHEMISTRY — CBGRC ROOM 1

8:00 S. Atkinson (Memorial University of Newfoundland): Study of Cationization of Glycine/1-Methyluracil Complexes Via Infrared Multiple Photon Dissociation Spectroscopy and DFT Calculations
8:15 S. Charoughchi (Concordia university): Cyclopropane-Core Based Molecules as Strong Electron Acceptors in Organic Semiconductors
8:30 T. Gong (York University): Electronic properties of anatase TiO_2 and iron (III) doped TiO_2 nanoparticles
8:45 S. Harroun (Université de Montréal): Using SERS and DFT to Examine Modified Nucleobases on Silver Nanoparticles
9:00 C. Hennecker (McGill University): Using transient equilibria (TREQ) to measure the thermodynamics of slowly assembling supramolecular systems
9:15 M. Keramatnejad (Concordia University): Impact of Pollutant Ozone on the Biophysical Properties of Tear Film Lipid Layer Model Membranes
9:30 H. Pham (McGill University): Unraveling the origins of strong and reversible chemisorption of carbon dioxide in a green metal-organic framework

BIOCHEMISTRY — CBGRC ROOM 2

8:00 L. Alagar Boopathy (McGill University): Study of the decay mechanism of HSP70 mRNA in Saccharomyces Cerevisiae
8:15 J. Allingham (Lakehead University): Brightening Up Brain Injuries: the Design, Synthesis and Characterization of a PET Diagnostic Agent for Neuronal Trauma
8:30 A. Aulakh (Simon Fraser University): Structural and functional studies of gypsy moth pheromone-binding proteins
8:45 D. Berry (McGill University): Characterizing NF1 Regulation of PD-L1
9:00 A. Blanchard (Université de Moncton): The Role of Mitochondrial Glycerol-3-Phosphate Dehydrogenase in Drosophila (Drosophila melanogaster) Acclimated to Different Temperatures.
9:15 A. Bouchard (UQAM): Novel molecular tools to increase SUMOylation of selected proteins
9.30 K. Chabi (UQAM): LC-MS/MS study of reactive metabolites formed by three estrogen analogues

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

ANALYTICAL CHEMISTRY — CBGRC ROOM 3

8:15 S. Ardalan (University of New Brunswick): Novelties in electrochemical platforms for rapid and in-situ diagnosis of Covid-19
8:30 O.-R. KUTEYI (Concordia): Stability of oxylipins on solid-phase microextraction devices
8:45 K. Krause (University of British Columbia): Toward the development of a quantum dot-based 'nose' for profiling protease activity
9:00 Y. Li (McGill University): Ag^+ Interference from Ag/AgCl Wire Quasi-Reference Counter Electrode Inducing Corrosion Potential Shift in an Oil-Immersed Scanning Micropipette Contact Method Measurement
9:15 E. Mariani (Concordia University): Characterization of phase two sulphonation reaction metabolites of 17 common mycotoxins

MOLECULAR BIOLOGY — CBGRC ROOM 4

8:00 M. Diawara (Université de Moncton): Creb1 et Cebpb, deux facteurs de transcriptions impliqués dans la régulation de l'expression de Sox9 dans les cellules de Sertoli du testicule adulte.
8:15 Y. Gu (McGill University): Emergence of β1 integrin-deficient mammary tumors from dormancy involves both epithelial cell intrinsic and extrinsic mechanisms
8:30 A. Gupta (Carleton University): Activation of the Hippo pathway in Rana sylvatica: yapping stops in response to anoxia
8:45 A. Ismailova (McGill University): The FoxP1/FoxP4 transcriptional network in inflammatory neutrophils
9:00 L. Kreps (Ottawa Hospital Research Institute; University of Ottawa): A Novel Xenograft Model of Metastatic Invasive Lobular Carcinoma
9:15 M. Ristovski (University of Ottawa): Speeding up Science: Predicting P4-ATPase Structures using UCSF Modeller
9:30 S. Selber-hnatiw (Concordia University): Secondary Metabolite Production in Aspergillus niger: methyltransferase specificity

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

INORGANIC CHEMISTRY — CBGRC ROOM 5

8:00 S. Christian-Robinson (Memorial University of Newfoundland): Biomass Adsorbent: Dye removal efficacy of self-assembled calcite
8:15 J. Hui (Concordia University): The effect of capping group swapping on perovskite nanocrystals
8:30 K. May (Ryerson University): An Investigation of Biologically Active Azole-Boron Containing Compounds (ABCC's)
8:45 M. Nayyar (Western University): Luminescent Group 11 Metal – Chalcogen Clusters with Conjugated Diphosphine Ligands
9:00 B. Rezaee (York University): Characterization and Electrocatalytic Performance of Amorphous Transition Metal Oxides
9:15 Z. Singh (Concordia University): Surface Grafting of a Donor-Chromophore-Acceptor Assembly onto Zinc Oxide Nanowires for Alcohol Oxidation
9:30 R. Brar (Concordia University): Studying energy transfer dynamics between Perovskite Nanocrystals and Coordination Compounds

SCHEDULE // TALK SESSION B // 11:15 AM – 12:45 PM EST

ENVIRONMENTAL & ANALYTICAL CHEMISTRY — CBGRC ROOM 1

11:15 Z. Aghaei (Memorial University of Newfoundland): Does exposure to microplastics during pregnancy impact fetal and placental development?
11:30 Y. Mirzaei (Concordia University): Exploring the Bacterial Preference in Degradation of Terrestrial and Marine Organic Matter of St. Lawrence Estuary by Stable Carbon Isotope Signature
11:45 L. Nguyen (University of Alberta): Mass spectrometry identifies sialoglycans as attachment factors of SARS-CoV-2
12:00 H. Parsimehr (University of New Brunswick): High-performance Electrocatalysts for Metal-Air Batteries.
12:15 E. Salehi Alaei (Western University): Evolution of Used Fuel Container Corrosion from Oxic to Anoxic Conditions
12:30 M. Mireault (UQAM): Metabolomic analysis of human urine and plasma by liquid chromatography-high resolution mass spectrometry

BIOCHEMISTRY & MOLECULAR BIOLOGY — CBGRC ROOM 2

11:15 F. R. Chowdhury (Concordia University): Controlling the evolution of antimicrobial resistance with collateral sensitivity loops
11:30 E. Digby (University of Toronto): Dark Dynamic Therapy: Photosensitization using a Dioxetane-Erythrosin B Conjugate
11:45 A. Erman (Carleton University): Investigating the effects of microRNA expression on the kidney of the thirteen-lined ground squirrel, Ictidomys tridecemlineatus, during torpor
12:00 M. Hemmings (McGill): Towards Structure-Guided Design of Aminoglycoside Phosphotransferase Inhibitors
12:15 F. Hunter-Manseau (Université de Moncton): The Importance of the Mitochondrial Unfolded Protein Response in the Fruit Fly (Drosophila melanogaster) During Nutritional Stress
12:30 H. Almousa (Concordia University): TRAPPC10 variants are associated with neurodevelopmental disorder and microcephaly in humans

SCHEDULE // TALK SESSION B // 11:15 AM – 12:45 PM EST

ORGANIC CHEMISTRY — CBGRC ROOM 3

11:15 D. Cadwallader (York University): Synthesis of Carbamoyl Fluorides with a Difluorophosgene Surrogate
11:30 H.-C. Chan (UQÀM): Copper-Promoted N-Arylation of the Imidazole Side Chain of Protected Histidine using Triarylbismuth Reagents
11:45 M. Chaudhry (University of British Columbia): Diverse binding modes of [3+3] Schiff-base macrocycles with ammonium guests
12:00 A. Cook (University of Ottawa): Nickel-Catalyzed Deoxygenation of Diverse C-O Bond-Bearing Groups: The Hunt for Potential Intermediates
12:15 M. Dashti (University of Windsor): Stimuli Responsive Triggered Self-immolative Pseudopeptides
12:30 M. Jafari (Concordia University): Conglomerate Crystallization Under the Influence of the Chirality Induced Spin Selectivity (CISS) Effect

COMPUTATIONAL CHEMISTRY — CBGRC ROOM 4

11:15 H. Mohamed (McMaster University): QSAR Model of EPAC1-Selective Modulators
11:30 S. Sharma (Blue Marble Space Institute of Science, Seattle, US): Computational Modelling of Prebiotic Autocatalytic Chemical Reaction Networks
11:45 S. W. Tatarchuk (University of Guelph): Mechanism of Urea Oxidation on β-$Ni(OH)_2$ from First-Principles Simulations

INORGANIC CHEMISTRY — CBGRC ROOM 5

11:15 N. Asok (York University): Structure-reactivity studies on hypervalent squarepyramidal dithieno[3,2-b:2',3'-d]phospholes
11:30 R. Carafa (Ryerson University): A Structural, DFT and Experimental Investigation of the Ring Stability and Ring-Opening Polymerization Behaviour of Cyclic Thionylphosphazenes in the Presence of Lewis Acid Catalysts
11:45 H.-V. Tran (INRS-Centre Armand-Frappier Santé Biotechnologie): Exploiting exo and endo furan-maleimide Diels-Alder linkages for the functionalization of organoruthenium complexes
12:00 M. Das Gupta (The University of British Columbia): Tunable Nanofibers from Benzene-1,3,5-Tricarboxamide Supramolecular Assemblies
12:15 N. Akter (University of Alberta): Self-Replicating DNA Based Nanoassemblies

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

PHYSICAL CHEMISTRY — CBGRC ROOM 1

13:30 S. Disanayaka Mudiyanselage (University of Saskatchewan): Probing the Photophysics Potentials of Azulene and Selected Azulene Analogues
13:45 A. E. Molina Lozano (Universidad de los Andes): Preliminary study of photoelectrochemical properties of cerium oxide-polyaniline photoelectrodes
14:00 M. Odetallah (University of Manitoba): The Electrode Microstructure Effect on The Battery Performance
14:15 H. Otani (University of British Columbia): Infrared spectroscopy of chiral molecules and their dimers in ultracold helium droplets
14:30 T. Shandro (University of Calgary): Got Gout? Utilizing peptide engineering to diagnose gout
14:45 Z. Zhang (McGill University): Adatoms in the surface-confined Ullmann coupling of phenyl groups.
15:00 O. Mohammadi (University of Saskatchewan): Ability of DNA Origami to increase Förster Resonance Energy Transfer (FRET)

BIOCHEMISTRY — CBGRC ROOM 2

13:30 S. Jacob-Tomas (McGill University): Using single-molecule fluorescence microscopy to uncover neuronal vulnerability to protein damage
13:45 P. Jaouen (Laval University): Interaction of S100B to cell membrane
14:00 J. Mohammed (McMaster University): Treatment of Bacterial Skin Infections Using Drug-Impregnated Polymer Hydrogels
14:15 F. Noël (Laval University): Influence of phospholipids on membrane binding of the S100A16 protein in the presence of calcium using Langmuir Monolayer Model and Biomolecular Modeling
14:30 M. R. Omrani (UQAM): Proteomics based screening of DDX3Y role in development of male-biased Hirschsprung disease
14:45 V. Pandya (Memorial University of Newfoundland): In-silico characterisation of the cryptic pocket inducing conformational transition in the human farnesyl pyrophosphate synthase
15:00 A. Shukri (Carleton University): Antimicrobial Resistance: Fighting back against Superbugs using systematic optimizations and degenerate peptide design

SCHEDULE // TALK SESSION C // 13:30 – 15:45 EST

ORGANIC CHEMISTRY — CBGRC ROOM 3

13:30 S. Eisinga (McMaster University): Chemically tuning covalent antibody recruiting molecules to modulate immune recognition and response: An application of sulfonyl fluoride exchange chemistry
13:45 R. Hernandez (Concordia University): A Scalable Desymmetrization of Poly(-ynes) By A Copper (II) Mediated Synthesis of 3,5- Disubstituted Isoxazoles Via 1,3-Dipolar Cycloadditions of Nitrile Oxides and Terminal Alkynes Under Planetary Ball-Milling Conditions.
14:00 S. Lacaille (Université de Montréal): Guanidine Derivatives and their Application Towards Pancreatic Cancer Treatment
14:15 J. Loos (University of British Columbia): Using molecular design to study the self-assembly of multicomponent low molecular weight gelators
14:30 A. McKnight (York University): Development Towards a Lewis Acid Catalyzed Intramolecular Acylfluorination Method
14:45 A. Pounder (University of Guelph): Intramolecular Nickel- and Palladium-Catalyzed Ring-Opening Reactions of Oxabicyclic Alkenes with C1-Tethered Aryl Halides
15:00 J. Price (University of New Brunswick): Predictable color-tuning in multicomponent photoluminescence systems & its application
15:15 K. M. Tam (McGill University): An Electrochemical Approach to Palladium-Catalyzed Carbonylative Coupling Reactions

BIOCHEMISTRY — CBGRC ROOM 4

13:30 S. Tijaro Bulla (University of Alberta): Modular Synthesis of a sgRNA for CRISPR-Cas9 Gene Editing
13:45 M. Tung (University of Toronto): Tellurophene-appended BODIPY: Photodynamic Therapy with Mass Cytometry
14:00 K. Turton (University of Lethbridge): The comparative biophysical characterization of the carboxysome and a minimal carboxysome
14:15 A. Van Kessel (McGill University): Live-cell monitoring of electrophile detoxification impairment during ferroptosis
14:30 R. Yu (Laurentian University): Investigate the regulatory roles of H_2S in lipid overload-induced lipotoxicity and cardiac cell senescence
14:45 J. Zhu (Laurentian University): H_2S reverses TNFα-induced MMP hyperactivity and elastin degradation in smooth muscle cells
15:00 S. Fonseca (Héma-Québec): Antibacterial Nanoparticle Coating: A Proactive Approach for Blood and Patient Safety

NANOCHEMISTRY — CBGRC ROOM 5

13:30 I. Abu-Baker (McGill University): Highly Organized Arrays of Gold Nanorings Assembled on Tobacco Mosaic Virus Coat Protein
13:45 D. Ali (Concordia University): Plant-derived phytoglycogen as a nanocarrier for the delivery of antimicrobial peptides
14:00 Y. Anisimov (University of Saskatchewan): Discerning the bonding in polyaniline-chitosan composites
14:15 K. Jeon (University of Toronto): Size-controlled synthesis of bioinspired polyserotonin nanoparticles with free-radical scavenging property
14:30 D. Mendoza (Concordia University): Development of Multimodal Imaging Probes Using Carbon Dots
14:45 H.-Y. Tsai (University of British Columbia): Toward Next-Generation Concentric Förster Resonance Energy Transfer Nanoprobes
15:00 A. Clermont-Paquette (Concordia University): Cellular uptake, cytotoxicity and trafficking of fluorescent carbon dots in human cells.

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

CBGRC ROOM 1

I01 - J.-L. Do (Concordia University, McGill University): Cavity-Containing Anionic Salicylic Acid-Based Metallostructures: Interplay Between Methylene and Aromatic Bridges in Ditopic Ligands
I02 - W. Leal (Concordia University): Conversion of electrochemically deposited carbonates to perovskite with retention of crystal morphology
I03 - A. MacKay (Concordia University): Arrested Development: Stabilization of an Aromatic Primary Hydroxylamine Function Upon Coordination with Transition Metal Ions
I04 - M. Molina (University of Calgary): Copper-MOF Electrocatalyst System for an Integrated CO_2 Capture and Conversion
I05 - S. Norouziyanlakvan (University of Ottawa): Electrocatalytic Generation of H_2 from Water with Zn(II) Complexes Displaying Cooperative Ligand Reduction
I06 - S. Thekkoot (York University): Cobalt based transition metal spinel oxide thin films as efficient water oxidation electrocatalysts
I07 - A. Watson (The University of Western Ontario): Exploring the Chemistry of Phosphorus Hydrazonides

CBGRC ROOM 1

O01 - Y. E. Augusto Jimenez (UQAM): Synthesis of analogues of PS–3114, a non-nucleoside inhibitor of DNMT3A
O02 - B. Cigana (Concordia University): Synthesis of Multi-Substituted Furans from Renewable Platform Chemicals.
O03 - M. Cyr (University of Ottawa): Exploring Ellagic Acid as an Organic Semiconductor
O04 - E. Hudson (University of Toronto): Synthesis of fluorescent analogues as mutated 1DH1 sensors for guided surgery of gliomas
O05 - S. Nadimi (university of Windsor): Diversifying the pseudoproline library to facilitate access to microcyclic peptides
O06 - T. Shao (University of Toronto): Metal Coordination of a Self-Assembling Histidine-Based Fatty Acid-Peptide Conjugate
O07 - K. Yeadon (Carleton University): Icephobic Coatings for Aerospace Applications
O08 - A. Fnaiche (UQAM): Development of New Small-Molecules TEAD Inhibitors Derived from Flufenamic Acid
O09 - S. Khan (Concordia University): Liesegang patterns of copper aspartate coordination polymer in gels

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

CBGRC ROOM 2

M01 - K. Bietar (McGill University): Effects of lanthanide-doped upconverting nanoparticles on nuclear biomarkers
M02 - Y. Chabi (Université du Québec à Montréal): Age-related neuronal changes, lifespan pathways and maintenance of neuronal architecture
M03 - S. Chu (McGill University): Cellular senescence impairs microtubule dynamics in intestinal epithelial cells
M04 - C. Lanteigne (Université du Québec à Montréal): The role of RNA decay and stability in dendritic spines development
M05 - H. T. Nguyen (Biology Department, Université de Moncton): JunB and Fra2 of the AP-1 transcription factors can regulate the expression of cadherin 3 in testicular Sertoli cells
M06 - M. PASCAL (Université du Québec à Montréal): Mechanisms of maintenance of nervous system architecture: role of the sax-7/L1CAM gene.
M07 - S. Rehman (Carleton University): Regulation of m6a related proteins during whole-body freezing of the wood frog, Rana sylvatica
M08 - R. I. Valette Reveno Leatis (Université du Québec à Montréal): Mechanisms regulating the extracellular matrix to ensure the long-term maintenance of neuronal organization and connectivity
M09 - R. Warkentin (Concordia University): Developing novel glycan binding proteins for tumor associated carbohydrate antigens by directed evolution

CBGRC ROOM 3

B01 - I. Ajala (Centre d'Excellence en Recherche sur les Maladies Orphelines Diseases- Fondation Courtois, and Biological Sciences department, Université du Québec à Montréal): Identification, subcellular localization and topology of AltSLC35A4, a highly abundant alternative protein in vertebrates
B02 - J. Arciszewski (McGill University): A new approach to plastic recycling: the use of enzymes in moist-solid reaction mixtures
B03 - B. Colalillo (McGill University): The Role of HuR in Adult T-Cell Leukemia/Lymphoma
B04 - L. Domínguez (Concordia University): Dynamics of the evolution of antibiotic resistance in soft agar
B05 - A. Harake (UQAM): Discovery of atypical SUMO E3 Ligases in humans through biochemical and bioinformatics approaches
B06 - F. Hutinet (Université du Québec à Montréal): Structural and molecular characterization of the interaction between SIZ1, a SUMO-E3 ligase involved in Arabidopsis thaliana environmental stress responses, and its substrates
B07 - K. Kethana (Diablo Valley College/Dougherty Valley High School): Optimizing Small-Molecule inhibition of Systemic Juvenile Idiopathic Arthritis (sJIA) and Macrophage Activation Syndrome (MAS) Biomarker Interleukin-18 (IL-18) via Autodock Vina and Swiss ADME
B08 - N. Kihal (UQAM): Amyloid peptide to guide the self-assembly of perylene diimide into functional nanostructures
B09 - P. Patel (McGill University): Systematic review of collagen biochemical properties in osteogenesis imperfecta
B10 - J. Plamondon (UQAM): Molecular tools to enhance protein SUMOylation: development and application in Rett Syndrome

B11 - M. Shred (McGill University): Drosophila Microtubule Dynamics Show High Rescue Rate and Low Nucleation Threshold
B12 - A. Varma (Carleton university): One step purification and regulation of fructose 1,6-bisphosphatase in the liver of freeze tolerant wood frog, Rana sylvatica
B13 - Y.Kim (University of Toronto): Acetylation of Hemoglobin and its effects on protein function and structure

CBGRC ROOM 4

E01 - S. Haghjoo (UNBC): Modification of NaA Zeolitized Coal Fly Ash with Hexadecyl Trimethyl Ammonium Chloride as a Novel Adsorbent for Glyphosate Removal
E02 - B. Keenan (McGill University): Fire history, vegetation and climate change in the Maya lowlands over 3,300 years
E03 - D. Alqdeimat (Memorial university): Ethanol fuel cell for clean environment
A01 - I. Benhadji Serradj (UQAM): Analyse des contaminants environnementaux dans les urines par LC-MRM
A02 - O. Zambito (UQAM): Untargeted metabolomic analysis of Hirschsprung's disease in a mouse model
N01 - K. Joshi (VN South Gujarat University, India): Review of current trends in Hydroxyapatite nano-particles for drug delivery applications – advantages and challenges
N02 - J. Chen (Université de Montréal): Polymer-Matrix Mediated Assembly of P3HT Nanowires
N03 - H. L. Nguyen (School of Chemical Engineering, Yeungnam University, 280 Daehak-Ro, Gyeongsan 38541, Republic of Korea): Powder X-Ray Diffraction Analysis of Cu/Cu2O Nanocomposites Synthesized by Colloidal Solution Method
P01 - S. A. Shobeiri (Memorial University of Newfoundland): Elucidation of proton dynamics and structure of an organic ionic plastic crystal employed in fuel cells using solid-state NMR
P02 - K. Snyder (University of Guelph): The Exploitation of Molecular Perturbation Effects in Experimental and Calculated Vibrational Spectroscopy
P03 - Z. Alinia (Concordia University): Phase behavior of 2D self-assembled phospole-lipid films

Study of Cationization of Glycine/1-Methyluracil Complexes Via Infrared Multiple Photon Dissociation Spectroscopy and DFT Calculations

S. Atkinson*, T. Fridgen
Memorial University of Newfoundland

Non-covalent binding drives vital interactions between biomolecules, ensuring selectivity during processes like DNA transcription or gene expression. This binding can be influenced by other ions or molecules to force tautomerization or cover binding sites, leading to different conformations and activity. The introduction of metals may be required for essential biomolecular features (zinc fingers), or otherwise result in detrimental or failed processes necessary for cell survival (heavy metal chelation). This study seeks to find the influence protonation and alkali metal cations have on the complexation of glycine and 1-methyluracil, both through IRMPD spectroscopy and comparison with low-energy geometry-optimized conformers calculated with B3LYP and M062X basis sets. Absorption bands explicate key structural features of the complexes, such as free O-H stretching and hydrogen-bonded intermolecular interactions.

Cyclopropane-Core Based Molecules as Strong Electron Acceptors in Organic Semiconductors

S. Charoughchi[1]*, H. Hase[2], P. Liu[3], M. Berteau-Rainville, P. Forgione[2], I. Salzmann[1]
[1]Concordia university, [2]Concordia University, [3]University of Toronto, [4]INRS

The p-doping of organic semiconductors (OSC), that is, conjugated organic molecules (COMs) and polymers (COPs), is generally done by using strong molecular acceptors as dopants. In principle, high doping efficiency is achieved with dopants of high electron affinity (EA) to promote electron transfer between COP/COM and the p-dopant. This leads to an increase in mobile charges in the COP/COM, which translates into an increase in conductivity. Common dopants (EA> 5) are typically lightweight, unstable, show low solubility in common solvents with most COPs/COMs, and tend to diffuse through the semiconductor host. Furthermore, their planarity can lead to the formation of ground-state charge transfer complexes (CPXs) with the COPs/COMs, which is detrimental to the doping efficiency. Recently, a new generation of dopants has been introduced based on a cyclopropane core such as hexacyano-trimethylene-cyclopropane (CN6-CP) of high EA (5.87 eV), which is highly unstable in air and therefore largely unsuitable for practical applications. Recent modifications of CN6-CP of still high EA have planar structures and are thus prone to promoting CPX formation.

This project explored the feasibility of different substitutions at the cyclopropane, such as pentafluorophenyl (PFP). This compound has been successfully synthesized and characterized regarding its structural, electronic, electrical properties.

Electronic properties of anatase TiO_2 and iron (III) doped TiO_2 nanoparticles

T. Gong*, S. Morin
York University

Since its discovery by Fujishima and Honda in 1972, titanium dioxide (TiO_2) has been studied extensively due to its ability to split water and decompose dyes as a photocatalyst.

Among all phases, TiO_2 in the anatase phase displayed the highest photocatalytic rates for dye decompositions. To maximize the efficiency of dye photodecomposition under solar light, iron is selected as the dopant to narrow the band gap from the UV towards the visible region. The dopant is non-toxic, abundant, and can enhance photodegradation rate as shown in previous studies.

We are proposing to use X-Ray Diffraction analysis, Scanning Electron Microscopy, Energy Dispersive X-ray spectroscopy to study nanoparticles prepared using the sol-gel method under different conditions, to confirm their phases, crystallite

sizes, morphologies, and average doping percentages. Moreover, to understand the effect of iron doping on photocatalytic properties, band gaps are measured via UV-Vis Diffuse Reflection Spectroscopy, and the valence band structure are obtained using X-ray Photoemission Spectroscopy and Ultraviolet Photoemission Spectroscopy. Models of electronic band structures of anatase phase TiO_2 with various iron doping percentages are proposed, and the theoretical effect of iron dopants on dye photodegradation rates are discussed using current experimental results.

Using SERS and DFT to Examine Modified Nucleobases on Silver Nanoparticles

S. Harroun
Université de Montréal

Surface-enhanced Raman spectroscopy (SERS) is mainly known as an analytical technique, whereby a target molecule's Raman signal is boosted via adsorption on a noble metal nanoparticle surface. Another application of SERS, however, is determination of the adsorption orientation of a molecule on the surface of the nanoparticles. Traditionally, this has been achieved by comparing the differences between the normal Raman and SERS spectra, whereas a more recent approach is to employ density functional theory (DFT) computations to elucidate the surface-adsorbed state. This is done by comparing various simulated spectra of the molecule interacting with the surface in different orientations, followed by determining which is most similar to the experimental spectrum. With an emphasis on analogues of the adenine nucleobase, this talk will cover a new approach that combines SERS with DFT, whereby tuning the surface properties used in the simulation can quantitatively improve agreement with experimental observations obtained on silver nanoparticle surfaces.

Using transient equilibria (TREQ) to measure the thermodynamics of slowly assembling supramolecular systems

C. Hennecker*, C. Lachance-Brais, H. Sleiman, A. Mittermaier
McGill University

Supramolecular chemistry involves the non-covalent assembly of monomers into materials with unique properties and wide-ranging applications. Thermal analysis is a key analytical tool in this field, as it provides quantitative thermodynamic information on both the structural stability and nature of the underlying molecular interactions. However there exist many supramolecular systems whose kinetics are so slow that the thermodynamic methods currently applied are unreliable or fail completely. We have developed a simple and rapid spectroscopic method for extracting accurate thermodynamic parameters from these systems. It is based on repeatedly raising and lowering the temperature during assembly and identifying the points of transient equilibrium as they are passed on the up- and down-scans. In a proof-of-principle application to the co-assembly of polydeoxyadenosine containing 15 adenosines (polyA) and cyanuric acid (CA), we found that roughly 30% of the CA binding sites on the polyA chains were unoccupied, with implications for high-valence systems

Impact of Pollutant Ozone on the Biophysical Properties of Tear Film Lipid Layer Model Membranes

M. Keramatnejad*, C. DeWolf
Concordia University

The tear film lipid layer (TFLL) is the outermost layer of the tear film and plays many important roles like reducing the surface tension of the tear film and helping with easy re-spreading after each blink. TFLL consists of a monomolecular layer of polar lipids creating the interface of the aqueous tear film with the multilayered formation of non-polar lipids, mostly cholesterol esters and wax esters which together compose up to 93% of the entire TFLL. Compromise in its composition and surface properties is one of the major reasons behind the prevalence of Dry Eye Syndrome, which is one of most common ophthalmic diseases today. Epidemiological studies have found an association between the increasing prevalence of Dry Eye Syndrome with environmental pollutants. Ozone has been of interest due to its oxidizing effect on the lipids. Being constantly exposed to environmental pollutants, such as ozone, TFLL can undergo compositional changes

that could be detrimental to the structure and the proper function of TFLL. Here we present our work on a model of TFLL using representative lipids of TFLL. We report the effects of multiphase reaction of ozone in relevant concentrations to environmental smog on the surface properties of our model membranes.

Unraveling the origins of strong and reversible chemisorption of carbon dioxide in a green metal-organic framework

H. Pham
McGill University

Cyclodextrin-derived metal-organic frameworks (MOFs) are remarkable not only because of their ability to absorb CO_2 strongly and reversibly but also because they can be readily obtained from inexpensive, renewable, and environmentally benign components. Despite the wealth of data on the carbon dioxide intake by CD-MOF-2, a representative of these MOFs, the nature and structural characteristics of its diverse adsorption sites, capable of binding CO_2 in the irreversible and reversible regimes, remains unclear. A comprehensive analysis of the results of the density functional theory modeling performed in this work in conjunction with experimental data shows that the hydroxyl counterions in CD-MOF-2 pull the protons away from the cyclodextrin alcohol groups, increasing their nucleophilic strength and turning them into strongly binding alkoxide chemisorption sites. At the same time, the diverse hydrogen bonding environments of the alkoxide sites reduce their nucleophilic character to a different extent, tuning their carbon dioxide binding to be irreversible, strong reversible, or weak. By linking the acid-base proton equilibrium and hydrogen bonding - two chemical concepts widely used for liquids - to the strength of the carbon dioxide binding in CD-MOF-2this work suggests new strategies for advancing design of tunable solid materials for carbon dioxide capture or detection.

Probing the Photophysics Potentials of Azulene and Selected Azulene Analogues

S. Disanayaka Mudiyanselage*, A. Stevens
University of Saskatchewan

Photovoltaics (PVs) are one of the crucial contributions from recent decades of research for efficiently converting solar energy into electrical energy. Present day PVs can achieve efficiencies of up to 30%. Singlet fission (SF) could further enhance the efficiency in OPVs via multiple exciton generation. SF is a photophysical downconversion process where initially a ground state chromophore is excited into a higher energy singlet excited state (S_1), and then two triplet states (T_1) excitations are produced by this chromophore sharing its excitation energy with a second ground state chromophore. Recent studies suggest that singlet fission can enhance efficiency up to around 50%. Azulene is a hydrocarbon that displays unusual photophysical properties. Azulene does not show SF although it satisfies the ideal energy gap requirements for SF. Azulene's unique energy level arrangement results in excitation-energy depletion by other fast competing pathways, like internal conversion instead of SF. Theoretically, electron-donating and electron-withdrawing substitution in selected positions of azulene will give rise to a significant difference in its energy gaps between its excited state and ground state which will promote SF. Consequently, I have analyzed the photophysics of four azulene derivatives 2-cyanoazulene, 1,3-dichcoloroazulene, 1,3-dichloro-2-tetramethylsilaneazulene, and 1,3-dicholoro-2-cyanoazulene and have compared their properties to azulene.

Preliminary study of photoelectrochemical properties of cerium oxide-polyaniline photoelectrodes

A. E. Molina Lozano
Universidad de los Andes

We show the partial results of the study of the photoelectrochemical properties of CeO_2 photoelectrodes in aqueous solution and its modification with PANI. In the first place, the results of the electrochemical synthesis of the oxide at constant potential are shown and a possible mechanism of its growth is explained. Then, the photoelectrochemical characterization of the oxides with and without temperature treatment is carried out and their photocurrent and photoresponse are compared and said results will be explained in terms of the behavior of the charge carriers in the oxide. Finally, the effects of the addition of PANI to the FTO structure are shown.

The Electrode Microstructure Effect on The Battery Performance

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[1]University of Manitoba, [2]university of Manitoba

The casting procedure of the electrode slurry, the slow agglomeration of the conductive additive, and the binder adhesive failure produce a non-uniform distribution of the electrode materials and the electrode's microstructural properties. As a result, an inhomogeneous electrode is produced, impacting the battery performance. It creates large verities in the local current density. It impacts ion and electron mobility, as well as the battery cycle life. [3,4]

The effect of the microstructure on the battery performance is not well understood yet. Therefore, different techniques have been developed to study the microstructure, each technique providing unique information.[5] Here, we will use scanning electron microscopy (SEM), four-point probe, and scanning electrochemical microscopy (SECM) in combination with battery cycling data to study the effects of the micro and macrostructure on battery performance.

SECM is a probe technique with nano-scale resolution, measuring the current or the potential of a substrate surface. Thus, we can measure the conductivity of the substrate's surface.[5,6] We will use this technique to find disconnected areas in the electrode and quantify the inhomogeneous distribution of the electrode`s microstructure. We combine this data with the data from cycling to find a correlation between the microstructure inhomogeneity and battery performance.

Infrared spectroscopy of chiral molecules and their dimers in ultracold helium droplets

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University of British Columbia

Our group investigate epichlorohydrin (ECH), a chiral halohydrin molecule, in He droplets with the goal of identifying chiral recognitions among the homochiral (*RR* or *SS*) or heterochiral (*RS*) pairs in an ultracold environment. Superfluid helium droplets consisting of several thousand helium atoms were generated by gas expansion at low temperature (10 K) and high pressure (20 atm) helium gas into a vacuum chamber. The droplets are known to be at 0.4 K due to evaporative cooling and to be able to pick up foreign molecules and separate them into the center of each droplet. By controlling the vapour pressure of the foreign molecules, the number of molecules in each droplet is precisely optimized. This technique is particularly useful to study molecular clusters such as dimers. Monomers and dimers of ECH molecules were picked up in helium droplets and their infrared absorption spectra were recorded in the 3 micron region utilizing a CW laser. The use of quantum chemical calculations and spectroscopy of ECH in a *para*-hydrogen matrix identified vibrational transitions of the ECH dimer and indicated slight spectral shifts from the monomer peaks. We are currently investigating the differences in the spectral features of the *RR* and *RS* dimers.

Got Gout? Utilizing peptide engineering to diagnose gout

T. Shandro
University of Calgary

Crystal arthropathies are forms of arthritis caused by the formation of crystals in the body, of which gout is the most prevalent. Sometimes called 'the disease of kings,' because it primarily affected the politically and socially powerful, gout can be triggered by a lifestyle of rich food and excessive alcohol consumption that was once affordable only by the affluent. However, gout is no longer restricted to the upper-class as the diet and lifestyle that predispose individuals to it have become increasingly common, and gout now affects 1-4% of adults in industrialized nations. Sufferers experience severe pain, redness and swelling of the affected region that negatively impacts the quality of life. Although it is one of the oldest recognized diseases, we lack fast, accurate tools to diagnose it, leading to the misdiagnosis and consequent

mismanagement of the disease. My research aims to develop a new technology platform using peptide engineering and basic fluorescence principles to accurately and selectively identify gout from other crystal arthropathies.

Adatoms in the surface-confined Ullmann coupling of phenyl groups.

Z. Zhang
McGill University

The on-surface Ullmann coupling of aromatic molecules has emerged as the most successful approach to synthesize atomically precise carbon nanostructures with unique electronic properties including molecular wires, graphene nanoribbons and two-dimensional conjugated polymers. Despite substantial progress in determining the mechanism of this reaction, the most fundamental question of whether the coupling is catalyzed directly by surface atoms or adatoms remains unanswered. In this work, the feasibility of the adatom creation and adatom-catalyzed Ullmann coupling of iodo-, bromo- and chlorobenzene on Cu(111), Ag(111) and Au(111) surfaces is examined using density functional theory modeling. Analysis of competing pathways reveals that two phenyl intermediates extract a silver atom from Ag(111) surface faster (energy barrier 0.43 eV) than they form the carbon-carbon bond (0.62 eV). However, on Cu(111) and Au(111), the extraction process is slower (0.71 eV Cu, 0.36 eV Au) than the C–C formation (0.49 eV Cu, 0.14 eV Au). The adatom creation is greatly facilitated by the strengthening of phenyl-metal bonds upon the extraction. Our results explain why adatoms are difficult to observe during surface-confined reactions and how their presence can lead to defects in the assembled nanostructures. The revealed trends can facilitate design of efficient on-surface reactions.

Ability of DNA Origami to increase Förster Resonance Energy Transfer (FRET)

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University of Saskatchewan

DNA origami, where origami refers to the art of Japanese paper folding, was first reported in 2006. DNA origami's self-assembly ability and easy procedure to create 2D and 3D structures with controllable geometry have motivated research towards its application in different areas. At the same time, scientists have been trying to improve FRET in light harvesting molecular systems. As it is a distance-sensitive energy-transfer process, it is important to finely control the distances between different types of dye molecules. My research focuses on designing and utilizing DNA origami as a platform to prompt efficient FRET by creating favorable molecular interactions. Using self-assembled DNA origami as a template for dye molecules allows us to control the precise arrangement and distance between these dyes. For instance, DNA origami can position dyes at distances of 3 nm. The results of this research will help us to develop fundamental knowledge about DNA origami and its application to improve FRET efficiencies.

ABSTRACTS // BIOCHEMISTRY ORAL PRESENTATIONS

Study of the decay mechanism of HSP70 mRNA in Saccharomyces Cerevisiae

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McGill University

The expression of the inducible HSP70 is tightly regulated. It is well known that under stress conditions the expression of HSP70 is transcriptionally activated by the Heat Shock Factor 1 (HSF1). During recovery, high levels of HSP70 inhibit HSF1 transcriptional activity by interacting with its transactivation domain. This negative feedback loop between HSP70 and HSF1 contributes to the repression of HSP70 transcription. Additionally, mRNA degradation prevents further HSP70 synthesis. It is reported that HSP70 mRNA is unstable and is degraded in a highly regulated fashion during recovery from stress. However, the molecular mechanism and regulators responsible for the efficient degradation of HSP70 mRNA is still unclear. We propose a link between HSP70 mRNA translation and decay as the mechanism mediating the efficient degradation and synchronous degradation of HSP70 mRNA during recovery from stress. We have characterized the decay

of HSP70 mRNA during recovery and identify components of the surveillance mechanism, No-Go Decay, regulating the fast degradation of the inducible HSP70 in Saccharomyces Cerevisiae.

Brightening Up Brain Injuries: the Design, Synthesis and Characterization of a PET Diagnostic Agent for Neuronal Trauma

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Concussions are an increasingly significant issue today, however, there is still no single standard, objective criterion for diagnosing them. The symptoms of concussions are often observed in the absence of significant structural damage making neuroimaging techniques such as computerized tomography and magnetic resonance imaging exceedingly difficult to use to identify their presence. An objective test with high sensitivity and specificity for concussions would provide a substantial advance in concussion diagnostics, which can help in the prognosis, treatment, and medical decision-making regarding the disorder. This research looks to fill the void in concussion diagnostic techniques by synthesizing a specifically designed, small molecule 18F-radiotracer capable of binding to a biomarker of neuronal trauma, thus allowing for imaging its upregulation using a PET scanner. The expression of S100B is upregulated in the presence of neuronal trauma events such as concussions. These increases correlate with astrocyte hypertrophy and proliferation as well as inflammation, thus S100B is a reliable biomarker of the onset and progression of astrogliosis in neuronal trauma and is the target of the 18F-radiotracer.

Structural and functional studies of gypsy moth pheromone-binding proteins

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Gypsy moths, Lymantria dispar, are considered destructive pests of hardwood trees. The caterpillars are voracious leaf eaters and cause major defoliations across Canadian forests. It has a chiral pheromone (7R, 8S)-epoxy-2-methyloctadecane, (+)-disparlure, that is highly attractive towards males, while (-)-disparlure is a behavioral antagonist. This remarkable enantioselectivity is encoded in the olfactory system of the moths. There is a need to understand, at the molecular level, their reproductive behavior to design an effective strategy in controlling their population. My work is focused on proteins called pheromone-binding proteins (PBPs) that are found in the male antenna and aid in transporting pheromones (released into the air by females) to the pheromone receptors. Activation of these receptors will produce neuronal signals directing the males in locating the females. There are two known PBPs in gypsy moth: LdisPBP1 and LdisPBP2. The mechanisms involved in PBP-pheromone binding and release are not yet known. We have studied the structure of LdisPBP1 by nuclear magnetic resonance (NMR) and the pheromone association and dissociation kinetics of both LdisPBPs. We will discuss the mechanism of ligand association and dissociation considering our structural work, and we will link the mechanisms to the function of PBPs in L. dispar pheromone olfaction.

Characterizing NF1 Regulation of PD-L1

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Immune evasion is a hallmark of cancer. Expression of immune checkpoint proteins, which include PD-L1 and CD80, mediate T-cell inhibition through binding to T cell receptors PD-1 and CTLA-4, respectively, to provide resistance to T cell killing. Immune checkpoint inhibitors (ICIs) are monoclonal antibodies that block these interactions to re-activate the anti-tumor immune response. ICIs have produced durable survival benefits for melanoma patients, quickly becoming the standard therapy for this malignancy. However, it is unclear why only a subset of patients respond to ICIs. Multiple sequencing studies have attempted to identify genetic alterations linked with response and resistance to ICIs. Recent studies have shown a correlation between mutations in the NF1 tumor suppressor and improved anti-PD-1 response. NF1 is an inhibitor of the RAS oncoprotein and is mutated in approximately 15% of melanomas. We have shown by co-immunoprecipitation and proximity ligation studies in melanoma cell lines that NF1 interacts with PD-L1. Importantly, we observed increased extracellular PD-L1 upon NF1 knock down in melanoma cells. These results support a model whereby NF1 forms a complex with PD-L1 to reduce its availability for interaction with T-cell PD-1 and immune evasion, which will have significant clinical implications for a number of NF1-mutant cancers.

The Role of Mitochondrial Glycerol-3-Phosphate Dehydrogenase in Drosophila (Drosophila melanogaster) Acclimated to Different Temperatures.

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Université de Moncton

The aerobic capacity of insects is essential to allow adaptation to temperature changes. In a previous study, we showed that the oxidation capacity of glycerol-3-phosphate (G3P) by the mitochondria was correlated with thermal tolerance in Drosophila. Therefore, we hypothesized that the mitochondrial glycerol-3-phosphate dehydrogenase (mG3PDH), allowing the oxidation of this substrate, might play a central role in thermal sensibility and temperature adaptation in Drosophila. We thus measured mitochondrial oxygen consumption at 15, 24 and 40°C (normal and critically high temperatures) in Drosophila acclimated to 15 and 24°C, gene expression of the mG3PDH, as well as resistance to cold (chill coma recovery) and to warm (heat tolerance assays) temperatures. Our preliminary results showed that Complex I mitochondrial respiration crashed at 40°C for Drosophila acclimated at 15 and 24°C. This was however compensated when G3P was added as a substrate, but only when flies were acclimated to 24°C. As expected, Drosophila acclimated at 15°C were less

heat tolerant and more resistant to cold. Finally, mG3PDH gene expression was significantly higher in flies acclimated to 15°C. Thus, our results showed that mG3PDH might be a necessary protein that controls metabolism during temperature adjustments and might be involved in temperature adaptation in insects.

Novel molecular tools to increase SUMOylation of selected proteins

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UQAM

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

LC-MS/MS study of reactive metabolites formed by three estrogen analogues

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UQAM

The metabolism of drugs contributes to their elimination by increasing their polarity. Unfortunately, some of these biotransformations can form reactive metabolites, which are linked to the toxicity of some xenobiotics. These reactive metabolites can bind to proteins and DNA, inducing severe cellular damage. A method often used for the characterization of these electrophilic species is based on the in vitro scavenging by glutathione, with the analysis of the formed adducts by liquid chromatography coupled to tandem mass spectrometry (LC-MS/MS).

In this study, we used isotope labeling combined with untargeted LC-MS/MS to comprehensively identify the reactive metabolites of three estrogen analogues. The metabolism of estradiol, estrone, and ethinyl estradiol was studied, as well as for their deuterated (d4) versions, using human or rat liver microsomal incubations. Four different trapping agents were evaluated, namely glutathione, N-acetyl-lysine and N-Boc-histidine and N-acetylcysteine. LC-MS/MS analysis and screening for isotope-labeled peaks allowed us to confirm known metabolites, as well as several previously uncharacterized metabolites. Adducts were studied by high-resolution MS/MS for structural elucidation. The use of isotope labeling also helped confirm the structures of many adducts.

Using single-molecule fluorescence microscopy to uncover neuronal vulnerability to protein damage

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McGill University

Neurodegenerative disorders (NDs) are diverse age-related conditions also described as “conformational diseases." The hallmark of NDs is the accumulation of disease-specific proteins as toxic misfolded aggregates in certain regions of the brain. They lead to the loss of protein homeostasis (proteostasis) that causes neuronal dysfunction and death. A potential therapeutic strategy for NDs is to prevent the accumulation of misfolded proteins through the activation of the heat shock response (HSR). However, how to manipulate the expression of HSPs to obtain a therapeutic effect in neurons remains unclear. The regulation of the HSR in neurons is more complex than what we have learnt from culturing non-neuronal cells. Here we describe a method to investigate the induction of HSP70 in primary hippocampal neurons using single-molecule fluorescence in situ hybridization (smFISH). Quantification of smFISH provides the means to analyze neuron-to-neuron variability in the activation of the HSR and to study the transcriptional induction and localization of HSP70 mRNA in primary neurons. This information might be critical to find the druggable steps for developing effective therapies to treat age-related NDs.

Interaction of S100B to cell membranes

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Laval University

Muller glial cells, located in the retina, are responsible for the physiological function of the eye nervous system. GC1 is an enzymatic transmembrane protein that transduces cell synaptic signals. The activity of GC1 is actually regulated by various proteins, including S100B in Muller glial cells. Thus, alterations in S100B function could deregulate GC1 synaptic transduction activity leading to ocular pathologies such as glaucoma, where loss of vision is observed. Yet no molecular information of S100B membrane interaction is known. Therefore, the study of membrane binding of S100B is key to understand the regulation of GC1 as well as its role in the retinal synaptic activity.

The goal of this research project is to characterize lipid membrane interactions of the retinal protein S100B. In this study, the Langmuir monolayer model was coupled to surface tensiometry in order to characterize the interactions between phospholipids and S100B in different experimental conditions.

The results obtained so far shows that S100B preferentially interacts with short, unsaturated acyl chains and phosphoethanolamine polar headgroups that are a major component of the Muller glial cell inner membrane. Furthermore, those lipids provide the membrane flexibility that may be necessary for synaptic transduction in Muller glial cells.

Treatment of Bacterial Skin Infections Using Drug-Impregnated Polymer Hydrogels

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[1]McMaster University, [2]Ceapro Inc

Open wounds are often a hotbed for bacterial infections and can pose a severe threat to individuals with compromised immune systems and other at-risk groups. Antibiotic-resistant bacteria, such as methicillin-resistant *Staphylococcus aureus*, thrive in these polymicrobial environments and are often difficult to treat. In addition to the ever-growing threat of antibiotic resistance, antibiotic compounds themselves often have inherent complications, such as low water solubility. As such, many drug candidates’ chemical and physical properties make administration challenging or even impossible. These challenges highlight the need for novel approaches to therapeutics and drug discovery and delivery. In collaboration with an Edmonton-based biotechnology company, Ceapro Inc., we propose a biopolymeric aerogel loaded with antibiotics of interest to address the solubility challenges associated with treating infected wounds. The bioaerogels are generated using pressurized gas expanded liquids (PGX), which increases the specific surface area in the gels by a hundred fold and therefore allows antibiotic loading by adsorptive precipitation. Using a clinically relevant mouse model, we develop tomorrows wound healing products by providing *in vivo* data to prove that these drug-impregnated PGX biopolymers improve the kinetics, localization, and efficacy of drug therapy for treating wound infections.

Influence of phospholipids on membrane binding of the S100A16 protein in the presence of calcium using Langmuir Monolayer Model and Biomolecular Modeling

F. Noël[1*], X. Yan[1], S. W. Vetter[2], É. Boisselier[1]

[1]Laval University, [2]North Dakota State University

Maintaining the structural and functional integrity of membranes is essential for proper cells function. A recent proteomic study suggests that S100A16 protein participates to the maintain of the membrane integrity in the rod outer segment (ROS) of the photoreceptors in the eye. The protein S100A16, recently discovered, is one of the S100 family proteins for which no protein and membrane interaction has yet been identified. Furthermore, maintain of the membrane integrity is a calcium sensitive process. The polar headgroup composition of the human ROS is 32.5% of phosphatidylcholine, 37.6% of phosphatidylethanolamine and 12.1% of phosphatidylserine. In addition, the polyunsaturated chains constitute between 30-60% of the total lipid fraction in humans. The cholesterol concentration of the discs varies from 32 to 5% between base and summit of ROS. The main objective consists of studying the membrane interactions of the S100A16 protein to better understand its function in maintaining membrane integrity. Specific objectives are: i) to gather information on its membrane interactions, and ii) to study the influence of calcium on these interactions. Langmuir monolayer model combined with surface tensiometry allows mimicking the composition of cell membranes and performing the membrane binding study. Biomolecular modeling will give complementary results of membrane interactions.

Proteomics based screening of DDX3Y role in development of male-biased Hirschsprung disease

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Hirschsprung (HSCR) disease is a developmental disorder of the enteric nervous system (ENS) due to failure of ENS progenitors in covering entire gut during embryonic development. HSCR is due to many gene defects, which are now identified at a steady pace. Yet, the reason why more boys than girls are affected by this disease remained very poorly understood. Our lab recently discovered that sequential upregulation of p53 protein activity and *Ddx3y* gene expression negatively impacts migration of neural crest-derived ENS progenitors and thereby promotes male-biased HSCR [Cardinal et al., PLOS Genetics 2020]. Intriguingly, this work notably showed that overexpression of *Ddx3y* alone did not have any impact on female ENS development, suggesting that DDX3Y acts in concert with other Y-linked genes. One candidate is *Eif2s3y*, which was found to be co-upregulated with *Ddx3y* in male *TashT* ENS progenitors. Current studies are now testing if DDX3Y and EIF2S3Y proteins directly interact in neural crest cells using BiFC. To identify other protein partners of DDX3Y, we have also initiated a proteomic-based screen using BioID. The new knowledge that will be gained through this work is expected to help the development of more efficient therapies for HSCR.

In-silico characterisation of the cryptic pocket inducing conformational transition in the human farnesyl pyrophosphate synthase

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Human farnesyl pyrophosphate synthase (hFPPS) is vital for numerous biological processes, controlling intracellular levels of farnesyl pyrophosphate. Bisphosphonate drugs are active site inhibitors of hFPPS that are valuable therapeutics to treat bone-resorption disorders and have also revealed efficacy in some tumour types. Continued drug discovery efforts led to the identification of monophosphonate compounds that inhibit hFPPS in a different mechanism. Crystallographic studies established that these inhibitors act by binding to an allosteric pocket found adjacent to the enzyme's active site. Recently, we have discovered a previously unidentified binding pocket in hFPPS, which appears to be better druggable than the allosteric pocket. Intriguingly, opening of the new pocket is observed only in the presence of a ligand that binds to the pocket and requires a conformational change that closes the allosteric pocket simultaneously. In the present study, we carried out extended molecular dynamics simulations of hFPPS for the following objectives: i) to understand the molecular mechanism underpinning the cryptic pocket-inducing conformational transition and ii) to capture the cryptic pocket in its most energetically favourable state. The latter objective, in particular, lays the groundwork for our future investigation that aims to develop potent cryptic pocket inhibitors of hFPPS.

Antimicrobial Resistance: Fighting back against Superbugs using systematic optimizations and degenerate peptide design

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There has been a marked increase in the resistance of bacterium to conventional treatments due to a misuse or overuse of antibiotics. There is, therefore, a need for the discovery and development of strategies to help alleviate antimicrobial resistance (AMR). Since their discovery, *β*-lactam antibiotics have been the first line of defense against AMR. Over time, resistance has been gained in clinical strains for a multitude of reasons, including the production of *β*-Lactamases (BLs) that metabolize these *β*-lactam antibiotics. As current antibiotics now demonstrate diminished therapeutic effects, there is a need for drugs that inhibit these mechanisms. To address this issue, this research uses peptide arrays to systematically develop new therapeutic peptides that overcome AMR. A protein fragment from a known BL inhibitory protein was systematically optimized with amino-acid permutations and tested for BL binding. Results from these experiments are then iteratively developed through multiple generations of peptide evolution. Once a defined list of BL-binding peptides is acquired, various assays will be performed to both characterize and elucidate the mechanism of inhibition between our target BL and our top scoring peptides. We plan to identify a list of peptides that will bind and inhibit BLs, identifying candidates for clinical research.

Modular Synthesis of a sgRNA for CRISPR-Cas9 Gene Editing

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Genome editing technologies are critical for both fundamental and applied research and are poised to make a significant clinical impact by reversing mutations in heritable diseases. In CRISPR/Cas9, the Cas9 endonuclease is guided to the correct DNA sequence through a guide RNA (gRNA). Chemical synthesis of single gRNAs is non-trivial because of the length of the RNA strand. Recently, we unveiled that a functional 97-nucleotide single gRNA (sgRNA) can be generated by stitching together three smaller fragments through a copper-catalyzed azide-alkyne cycloaddition. The primary advantage of this modular synthesis is that each of the strands are more manageable in size, thus enabling chemical modifications to be more easily incorporated. Two chemical modification that we have pursued are fluorophores for enabling fluorescence-assisted cell sorting (FACS) and chemical modifications for enhancing stability. Here, we demonstrate the synthesis of a sgRNA containing 2'-O-methyl-modified phosphorothioate nucleotides at both ends of the strand, which greatly increases successful gene editing in cells. Ongoing efforts are implementing this approach to better facilitate multigene editing and homologous directed repair (HDR).

Tellurophene-appended BODIPY: Photodynamic Therapy with Mass Cytometry

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Photodynamic therapy (PDT) is a clinically approved cancer treatment that utilizes photosensitizers (PS), which are light-responsive molecules that can produce cytotoxic reactive oxygen species (ROS) to treat diseases. In addition to treatments, PSs are also capable of diagnostics (i.e., theranostics) as many can fluoresce as well as generate ROS. However, since the mechanisms for fluorescence and ROS production compete in a light-absorbed, excited PS, photochemically tuning PSs to have suitable ROS and fluorescence quantum yields can be challenging. Herein, we describe the synthesis and characterization of a tellurophene-appended BODIPY, a compound detectable by mass cytometry (MC) and is capable of generating ROS. By introducing a tellurium atom, a fluorescent BODIPY dye is converted into a potent PS and acts as a mass tag to enable detection by MC. Our compound was found to be effective against HeLa cells with nanomolar IC_{50} and its presence in cells was confirmed by MC. This work describes a promising strategy for generating alternative theranostic PSs by coupling PDT with MC and future studies will include introducing selectivity towards target cells such as cancers so that MC can be used to monitor its accumulation.

The comparative biophysical characterization of the carboxysome and a minimal carboxysome

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Protein cages or protein nanocompartments (PNCs) are being increasingly used for biotechnological applications such as drug delivery, vaccine development, and agriculture. Most PNCs can efficiently store specific cargos, have protective characteristics against environmental conditions, and can be modified to cater specific usage. The carboxysome, a large bacterial microcompartment (BMC), is like many protein cages as its proteinaceous shell is used for the compartmentalization of proteins and small molecules. This BMC naturally stores large concentrations of cargo, Ribulose-1,5-bisphosphate carboxylase-oxygenase (RuBisCO), as well as its substrate, carbon dioxide, to provide high enzymatic activity of the protein RuBisCO. Despite the potential for the carboxysome to be used in biotechnology applications, its complexity has limited its implementation. Recently, "minimal carboxysomes" have been produced, as they may be easier to implement in biotechnological applications. The goal of this study is to use biophysical methods to characterize the carboxysome and minimal carboxysome structures and the abundance of different species *in vitro*. Our aim is to not only define the experimental methods that can be used to easily characterize these structures but to also determine the diversity of carboxysome species to optimize its use in different applications.

Live-cell monitoring of electrophile detoxification impairment during ferroptosis

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The mechanism linking iron-dependent lipid hydroperoxide (LOOH) accumulation and membrane permeabilization during ferroptosis, a recently described cell death pathway, is poorly understood. Here, we present studies conducted of live cell undergoing ferroptosis that establish LDE detoxification impairment associated with electrophile accumulation as a hallmark of ferroptosis downstream of LOOH accumulation. We developed an assay utilizing a fluorogenic lipophilic electrophile (AcroB) that, in combination with an aldehyde-reactive probe, enabled assessment of i. the glutathione-mediated LDE conjugation and adduct export steps of the LDE detoxification pathway and ii. the level of electrophile accumulation in live cells during ferroptosis. Importantly, targeted exacerbation of LDE-adduct export immpairment greatly increased ferroptosis susceptibility. Our results position the LDE detoxification pathway as a defense mechanism to prevent or delay cell death following ferroptosis induction and the failure of this pathway as a critical step during ferroptotic cell death. Our findings expand ferroptosis research downstream of LOOH accumulation towards unraveling the full molecular mechanism of this form of programmed cell death.

Investigate the regulatory roles of H2S in lipid overload-induced lipotoxicity and cardiac cell senescence
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Laurentian University

Hydrogen sulphide (H2S) is now recognized as a third gaseous mediator along with nitric oxide and carbon monoxide. H2S can be endogenously produced from cysteine in our body, and cystathionine gamma-lyase (CSE) acts as a major H2S-generating enzyme in the cardiovascular system. Increasing evidence has demonstrated that disturbed H2S production is relevant to heart disorders. This study investigated the regulatory roles of the CSE/H2S system on lipid overload-induced lipotoxicity and cardiac senescence. Here, it was found that incubation of H9C2 (rat cardiomyocyte cells) with lipid mix inhibited cell viability and promoted the cellular accumulation of lipid, generation of reactive oxygen species (ROS), mitochondrial dysfunctions, and lipid peroxidation, all of which could be reversed by incubation with exogenously applied NaHS (an H2S donor). Further data revealed that H2S protected H9C2 cells from lipid overload-induced senescence by altering the expressions of lipid metabolism-related genes and inhibiting the generation of acetyl-CoA and the level of global protein acetylation. In vivo, knockout of the CSE gene strengthened cardiac lipid accumulation, protein acetylation, and cellular ageing in high fat diet-fed mice. Taken together, the CSE/H2S system is essential for maintaining lipid homeostasis and cellular senescence in heart cells under lipid overload.

H_2S reverses TNFα-induced MMP hyperactivity and elastin degradation in smooth muscle cells
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Laurentian University

Enzymatic degradation of elastin by matrix metalloproteinases (MMPs) leads to the degeneration of aortic wall and constitutes the most prominent characteristic of aortic aneurysm. Hydrogen sulfide (H_2S) as a new gasotransmitter exhibits a wide variety of cardio-protective functions through its anti-inflammatory and anti-oxidative actions. However, the regulatory role of H_2S on elastin homeostasis has not yet been explored. Here we found that an active inflammatory cytokine TNFα induced MMP2/9 hyperactivity and elastin degradation in cultured smooth muscle cells, which could be reversed by overexpression of cystathionine gamma-lyase (CSE, a major H_2S-generating enzyme) or exogenously applied H_2S at physiological relevant concentration. In contrast, knockout of CSE deteriorated TNFα-induced MMP2/9 hyperactivity and elastin degradation. Either TNFα or H_2S had no effect on the mRNA or protein expressions of MMP9, cathepsin G/K, TIMP1, and elastin homeostasis-related proteins, while H_2S reduced MMP2 transcription. It was further showed that H_2S inhibited MMP2 promoter activity by posttranslational modification of Sp1 via *S*-sulfhydration. H_2S also directly attenuated MMP hyperactivity by *S*-sulfhydrating at the cysteine switch center. Taken together, this study suggests that CSE/H_2S system can be a new therapeutic avenue for the prevention and treatment of aortic aneurysm.

Antibacterial Nanoparticle Coating: A Proactive Approach for Blood and Patient Safety
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Introduction: A proactive approach to prevent infections associated with contamination from medical devices is based on the application of a Medical Antibacterial and Antiadhesive Coating (MAAC). Given that its antibacterial activity had already been demonstrated, the main objective of this project was to assess the MAAC antibacterial properties in complex blood product matrices.

Methods: The MAAC was deposited on plasticized PVC sections (dMAAC ~50 µm) obtained from red cell concentrate (RCC) and platelet concentrate (PC) bags. The adhesion properties of PVC ± MAAC were characterized by electron microscopy. The antibacterial activity of PVC MAAC was tested in accordance to ISO 22196:2011 standards against selected bacterial species in the presence of whole blood, or blood components, for Δt = 24 h (n=3).

Results: The number of S. aureus adhered to the PC and RCC PVC have decreased by 63% and 99% respectively after a 24h contact period in nutrient broth. PVC MAAC exhibited no significant antibacterial activity for any of the bacterial strains tested in RCC and PC, compared to the 1 to 4 log reduction previously obtained in nutrient medium. Tests with

separated blood components have shown that the absence of antibacterial effect seems to be mainly linked to high cellular densities or plasma protein concentrations.

Conclusions: This study demonstrates how the MAAC can prevent bacterial contamination in specific conditions, but more extensive data are yet to come for blood component applications.

ABSTRACTS // ANALYTICAL CHEMISTRY ORAL PRESENTATIONS

Novelties in electrochemical platforms for rapid and in-situ diagnosis of Covid-19

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It has been about two years since the Coronavirus disease 2019 (Covid-19) pandemic has cast a shadow over people's health and global economics. Reverse Transcriptase Polymerase Chain Reaction (RT-PCR) has been introduced as the gold standard biochemical analysis of Covid-19 causative virus's genetic materials, namely SARS-CoV-2 mRNA and its spike proteins. Although RT-PCR is a powerful technique for sensitive and accurate diagnosis of Covid-19, its drawbacks such as long analysis time, costs, need for trained personnel for sampling, sample preparation, and advanced instrumental analysis have resulted in poor efficiency when mass testing is required. Herein, emerging electrochemical technologies for rapid, point-of-care (POC), and situ detection of SARS-CoV-2 will be introduced, including the advancements in classical immunosensors, artificial bioreceptor-based biosensors, CRISPR-based molecular circuits, field-effect transistor-based biosensors, and multiplex platforms. The fundamental mechanisms of such novel biosensors will be introduced, and it will be explained how these novel platforms can facilitate accurate and efficient mass testing. Moreover, the challenges that may impede the commercialization of the novel POC platforms will be discussed as well as the probable solutions to tackle such challenges.

Stability of oxylipins on solid-phase microextraction devices

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The stability and accurate measurement of oxylipins in biological fluids and tissues are critically important in clinical and biomedical research since they are involved in inflammation and pain. Oxylipins can degrade due to oxidation, hydrolysis and isomerization as well as enzymatic conversion. In vivo solid-phase microextraction (SPME) is an extraction technique that was recently introduced for the quantification and profiling of oxylipins in brain tissue. These devices do not co-extract proteins from the sample, thus eliminating the enzymatic conversion of oxylipins during sampling, storage, and sample preparation. This study aims to investigate the on-device oxylipin stability to non-enzymatic degradation during the freeze and thaw process and prolonged room temperature storage. 46 oxylipin standards were extracted using HLB SPME devices. All samples were analyzed using C18 liquid chromatography-high resolution mass spectrometry. The results of freeze and thaw experiments were compared against control freshly prepared samples analyzed immediately after preparation (t=0). Using the 80-120% acceptance criteria and ANOVA statistical analysis, 11β-prostaglandin F2α, 13-hydroxy-docosahexaenoic acid, 9-hydroxyoctadecadienoic acid, and prostaglandin F2 were found to be unstable after 2 freeze-thaw cycles. This is the first time that the oxylipin stability on SPME devices has been characterized and shows how SPME may successfully improve their stability.

Toward the development of a quantum dot-based 'nose' for profiling protease activity

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Proteases play a vital role in human health: there is thus demand for assays to detect abnormal protease activity for disease diagnosis. However, it can be challenging to profile protease activity using conventional assays, particularly when the identity of the disease-causing protease(s) is unknown. Chemical noses detect analytes based on patterns of signals from non-specific sensors. This non-specificity enables classification of samples containing analytes outside of the training set, which can facilitate categorization of samples without knowing the target analyte. Quantum dots (QDs) are ideal platforms for chemical noses, as their readily tunable surface chemistry can provide a basis for non-specific analyte-sensor interactions.

Here, we present research toward a QD-based nose that can differentiate a dozen serine proteases. Sensor elements consist of QD-peptide conjugates with different combinations of peptides and surface chemistries. QD surface chemistry significantly impacts proteolytic rates, and we have systematically studied the effect of a range of small-molecule and polymeric QD ligands on proteolytic rates to develop the nose. In addition to the nose's significance as a sensitive, multiplexed assay for protease activity, the nose also represents a proof of concept of the ability of QD surface chemistry to differentiate between enzymes.

Ag^+ Interference from Ag/AgCl Wire Quasi-Reference Counter Electrode Inducing Corrosion Potential Shift in an Oil-Immersed Scanning Micropipette Contact Method Measurement

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The commonly used Ag/AgCl wire quasi-reference counter electrode in the miniaturized electrochemical cell of the scanning micropipette contact method (SMCM) was found to leak Ag^+ into the electrolyte solution, bringing deleterious effects on quantitative measurements. The reduction of these Ag^+ species at the working electrode surface generated a faradaic current, which significantly affects the low magnitude currents inherently measured in the scanning micropipette contact method. We demonstrate that, during the microscopic corrosion investigation of the AA7075-T73 alloy using the oil-immersed SMCM, the cathodic current was increased by the Ag^+ reduction, resulting in positive shifts of corrosion potentials. The use of a leak-free Ag/AgCl electrode or extending the distance between the Ag/AgCl wire and micropipette tip eliminated the Ag^+ contamination, making it possible to measure accurate corrosion potentials during the oil-immersed SMCM.

Characterization of phase two sulphonation reaction metabolites of 17 common mycotoxins

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Mycotoxins are toxic secondary metabolites that contaminate foods which pose a health risk to animals and humans. Current analytical methods to determine human exposure to these mycotoxins primarily focus on the detection of the parent compound. This can lead to underestimation of exposure levels, so it is important to determine the mycotoxin metabolites formed. Therefore, the objective is to perform sulphonation metabolism using human microsomal incubations on mycotoxins from zearalenone, trichothecene and aflatoxin classes and characterize the metabolites formed. The incubations were performed using S9 liver microsomal fractions and 3'-phosphoadenosine-5'-phosphosulfate. High concentration of mycotoxin (1 µg/ml) were used to permit the detection of the minor sulphates formed. Samples were analyzed using a highly-sensitive liquid chromatography-high resolution mass spectrometry (LC-HRMS) method and pentafluorophenyl column previously validated for the chosen mycotoxins in human plasma. The metabolites were characterized using accurate mass, MS/MS, and MS3 fragmentation. An in-house spectral library was built to aid in future exposure analysis studies and contains the characterized metabolites with their mass spectral information. For the zearalenone class all the expected metabolites were detected. Sulphonation after phase I metabolite formation was monitored and many minor metabolites were detected. Lastly, 15-acetyldeoxynivalenol showed two metabolites which has not been reported.

Creb1 et Cebpb, deux facteurs de transcriptions impliqués dans la régulation de l'expression de Sox9 dans les cellules de Sertoli du testicule adulte.

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Selon Santé Canada, 1 couple sur 6 au Canada est touché par l'infertilité. Cette infertilité est à 30% attribuable à l'homme. Les causes peuvent être diverses d'où l'intérêt de mieux comprendre les mécanismes de régulation de l'expression des gènes chez les cellules des testicules. Dans ces derniers se trouvent les cellules de Sertoli qui soutiennent la spermatogenèse. La régulation de ces cellules fait intervenir plusieurs gènes dont les gènes Sox qui sont exprimés de façon spécifique au cours de la différenciation et du développement. Au stade embryonnaire, l'expression de Sry conduit à la différenciation des cellules progénitrices de Sertoli. Sry active l'expression du gène Sox9 et à partir de ce stade du développement, l'expression de Sox9 est restreinte aux cellules de Sertoli et se maintient durant l'âge adulte. Par contre, les profils des facteurs de transcription de ces deux stades de développement sont distincts. Notre hypothèse est que le promoteur du gène Sox9 possède des séquences régulatrices qui vont permettre le recrutement d'autres facteurs régulateurs afin de maintenir son expression chez les cellules de Sertoli adultes. À cet effet, nous allons nous intéresser à la régulation de l'expression de Sox9 par Cebpb et Creb1 dans ces cellules de Sertoli adultes.

Emergence of β1 integrin-deficient mammary tumors from dormancy involves both epithelial cell intrinsic and extrinsic mechanisms

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The molecular and cellular mechanisms behind mammary tumour dormancy are unclear and how these processes are dynamically orchestrated to allow for tumor resurgence remains to be elucidated. In concordance with our previous studies, we report that mammary epithelial specific disruption of β1 integrin in a murine model of Luminal B human breast cancer drastically impairs tumour growth. This phenotype is accompanied with proliferation block, apoptosis induction and cellular senescence, altogether resulting in tumour mass dormancy. Molecular analyses from the sequencing of β1 integrin-deficient dormant lesions show activation of p53 tumour suppressor, and tumours that eventually escape dormancy possess mutations in such pathway analogous to that in human disease. We further demonstrate that mammary epithelial deletion of p53 in β1 integrin-deficient mice fully rescues dormant tumour phenotype and bypasses cellular senescence. Additionally, recurrent β1 integrin-deficient tumors exhibit fibrosis with increased cancer-associated fibroblast infiltration and extracellular matrix deposition, absent in fast-growing p53/β1 integrin-deficient lesions. Taken together, these observations argue that β1 integrin modulates p53-dependent cellular senescence resulting in tumor dormancy and that pro-tumorigenic stromal cues and intrinsic genetic mutation are required for dormancy exit.

Activation of the Hippo pathway in Rana sylvatica: yapping stops in response to anoxia

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Rana sylvatica display well-developed anoxia tolerance as one component of their capacity to endure prolonged whole body freezing during the winter months. Under anoxic conditions, the animal efficiently cope with stress by suppressing global gene transcription and promoting activation of mechanisms that support cell survival. Activation of the Hippo signaling pathway initiates cascade of protein kinase reactions that end with phosphorylation of YAP protein. Multiple pathway components of the Hippo pathway were analyzed via immunoblotting, qPCR or DNA binding ELISAs to assess the effects of 24 H anoxia and 4 H aerobic recovery, compared with controls, on liver and heart metabolism of wood frogs. Immunoblot results and transcript levels showed significant increases in the relative levels of multiple proteins of the

Hippo pathway. Decrease in YAP and TEAD protein levels in nuclear fraction also confirmed this. DNA binding activity of TEAD at the promoter region and changes in the protein levels of OCT4 and SOX2 suggested repression of gene transcription. Increased levels of TAZ in anoxic hearts suggested its involvement in the repair mechanism during anoxia. In summary, this study provides first insights into the role of the Hippo pathway in maintaining cellular homeostasis in response to anoxia in amphibians.

The FoxP1/FoxP4 transcriptional network in inflammatory neutrophils

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Neutrophils, the most abundant leukocytes, deploy an antimicrobial response against pathogens through release of pro-inflammatory cytokines. Defective neutrophil antimicrobial processes contribute to infection and chronic inflammation. Understanding (de)regulated transcriptional networks in neutrophils is crucial for gaining insight into responses to infectious or inflammatory signals.

To this end, we carried out the first RNA-sequencing analysis of human neutrophils treated in the presence or absence of bacterial lipopolysaccharide (LPS). Through a bioinformatic meta-analysis of our data and previously published smaller studies of LPS-stimulated neutrophils, we identified the most enhanced transcriptional network driven by the Forkhead Box transcription factor FoxP1, likely as a heterodimer with FoxP4. The network is enriched in genes that encode cytokines and inflammation-induced transcription factors, such as MAFF and ATF3. We report increased expression of FOXP1 and FOXP4 in LPS-treated neutrophils at the gene and protein level. Furthermore, we found FoxP1/4 binding sites within several genes in the network, all located in regions consistent with neutrophil enhancer function.

We are currently examining the interaction of FoxP1 and FoxP4 with the putative binding sites by chromatin immunoprecipitation (ChIP) and reChIP assays. We anticipate that the network exerts a profound effect on downstream gene expression, cytokine release and ensuing neutrophil function.

A Novel Xenograft Model of Metastatic Invasive Lobular Carcinoma

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lleInvasive lobular carcinoma (ILC) accounts for approximately 10% of invasive breast cancer incidences and is drastically understudied compared to its counterpart, invasive ductal carcinoma (IDC). Research on advanced disease in patients with ILC has been impeded due to a lack of invasive ER+ ILC cell lines and metastatic in vivo models. To meet this need, we have isolated ILC cells which show invasive and metastatic characteristics in vivo, thus presenting a novel ILC orthotopic xenograft model. MDA-MB-134VI is a representative ER+/PR-/E-cad- human ILC cell line which was allowed to invade for 7-days through Matrigel-coated transwells, and invaded cells (VIVA1) were isolated and expanded. VIVA1 cells were injected intraductally into mice to assess tumour growth in vivo. VIVA1 cells exhibited similar tumour growth and survival kinetics to the parental MDA-MB-134VI line, however unlike MDA-MB-134VI, the VIVA1 cells produced macrometastases in 6/10 animals. Tumour cells were isolated from primary tumors in the orthotopic site (VIVA-LIG43) and these were re-injected intraductally. VIVA-LIG43 cells had faster tumour onset and growth rate in the mammary ducts than the parental VIVA1 cells. We have created a novel orthotopic xenograft model of metastatic ILC, which provides researchers with a model for investigation of mechanisms driving ILC metastasis.

Speeding up Science: Predicting P4-ATPase Structures using UCSF Modeller

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University of Ottawa

Type-IV ATPases, or P4 ATPases are essential membrane proteins in maintaining lipid homeostasis of living organisms. The objective of this study is to exploit the homology modelling approach and investigate the predicted conformational changes of four novel members of P4-ATPases. We have used UCSF Modeller to generate theoretical models of four P4-ATPase homologs (ATP10A, ATP10D, Dnf1, and Neo1). Further, residues carrying human disease mutations and loss-of-function mutations in yeast will be examined in order to predict how mutants may affect the structural changes among different conformational intermediates. These models will be used as logical designs of site-directed mutagenesis for functional analysis using recombinant proteins. The models will be visualized using molecular graphic software such as Pymol. To generate homology models, we have first performed multiple sequence alignments by bioinformatic approaches, followed by in silico simulation of each P4-ATPase homolog. The best models were selected based on the lowest energy minimization out of 100 simulated models. The results of this study will be used in the future as theoretical models in comparison with the experimental data by either X-ray crystallography or cryo-electron microscopy. Ultimately, the study aims to elucidate the structure-function relationship of the P4-ATPase phospholipid transporters.

Secondary Metabolite Production in Aspergillus niger: methyltransferase specificity

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Secondary metabolites (SM) are compounds not directly involved in the growth or viability of an organism, but represent a source of pharmacologically or industrially relevant compounds that provide a selective advantage. Using the fungal genetic toolbox in Aspergillus niger, biosynthetic gene clusters (BGCs) controlling the synthesis, chemical modification, and transport of backbone enzymes in SM production can be manipulated. The BGC producing neurokinin receptor antagonist BMS- 192548 is tautomerized from the neuropeptide Y antagonist TAN- 1612 through an O-methyltransferase tailoring enzyme that regulates the selective addition of methyl groups. Methyltransferase specificity is important to our understanding of redesigning molecules, in which the product of altered methylation may lead to pharmacologically or industrially relevant SMs. In this work we aim to replace the native methyltransferase with candidate methyltransferases present in the A. niger genome and analyse the resulting methylation pattern. BGC engineering and SM profiles of the mutant strains will be presented.

Biomass Adsorbent: Dye removal efficacy of self-assembled calcite

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Dyes in wastewater streams from paper, clothing, etc., industries are worrying due to their persistence and the high level of risk posed to the environment. Several methods have been utilized to remove these contaminants from wastewater systems, with the most widely employed being adsorption by activated charcoal. However, activated charcoal is affected by high production costs and a low degree of regeneration. As a result, alternative biomass-derived materials are increasingly being studied. In this presentation, a sponge-like material termed self-assembled calcite (SAC), made from blue mussel shells, is investigated for its potential in dye wastewater treatment processes. Batch adsorption experiments were set up with methylene blue (MB) dye concentrations 5.01, 7.51, 10.02, 12.52, 15.02, 17.53, 20.03 mg/L, each with 0.5 g of SAC. After a 48 hours equilibrium, a maximum adsorption percentage of 81.83% was reached for the 5.01 mg/L sample. The results from the batch studies were fitted to the Langmuir adsorption isotherm and gave a maximum adsorption capacity (qm) of 1.7718 mg/g. From calculations of the separation factor (RL), the overall adsorption process of MB onto SAC was deemed favorable.

The effect of capping group swapping on perovskite nanocrystals

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Perovskites are a material of emerging interest with many potential uses such as LEDs and photovoltaics. Having the general formula ABX3 (A = cation, B = cation, X = anion) they are known for their highly tunable bandgap, easy synthesis and have shown great promise for solar energy conversion, although their devices are limited by degradation when exposed to ambient condition such as air and moisture. This work describes following a known hot injection method for the synthesis of CsPbBr3 nanocrystals, an ion-exchange method for CsPbCl3, CsPbI3 and through ligand exchange, parent capping groups (oleic acid and oleylamine) are replaced by fluorinated benzoic acid derivatives. This project follows this step closely to determine the effect that this swap may have on the perovskite nanocrystal via the analysis of NMR, photoluminescence, quantum yield, lifetime, FT-IR, and TEM in hopes these substitutions bring about a new route for further application of these materials.

An Investigation of Biologically Active Azole-Boron Containing Compounds (ABCC's)

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Prior to 2003, boron-containing compounds (BCC's) were mostly overlooked when considering functionality for drug design. Since the FDA approval of Bortezomib (Velcade - a peptide-mimic drug) the field of medicinal Boron based drugs has blossomed as BCC's have seen increased use and research interest in pharmaceuticals. Having a particularly high affinity for oxygen, boron-oxygen chelated complexes and boronic acid esters have been increasingly popular in recent BCC's. We are interested in the development and characterisation of N,O- and N,C-chelates of BCC's and their potential as biologically active species. We intend to take advantage of the known biological activity of which oxazolines, oxazoles and thiazoles display and use them in tandem with those of the boron center to hopefully increase biological efficacies.

Advancements towards the synthesis of various ligands scaffolds as well as future directions to ascertain their biological activity will be discussed.

Luminescent Group 11 Metal – Chalcogen Clusters with Conjugated Diphosphine Ligands

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The bidentate phosphine 4,6 – bis(diphenylphosphino)dibenzofuran (dbfdp) has been employed recently as a ligand for the assembly of highly luminescent Cu_4I_4 cubane clusters and these have been incorporated into organic light emitting diode (OLED) devices. Our recent work focuses on using dbfdp and related substituted diphosphines for the controlled assembly of group 11 metal – chalcogen (S, Se, Te) clusters and an investigation of their luminescent behaviour.

To this end, the dbfdp ligand can be reacted with CuOAc or AgOAc to form the dimeric $[\{Cu(OAc)(\text{-dbfdp})\}_2]$ and $[\{Ag(OAc)(dbfdp)\}_2]$. These are excellent precursors for the facile preparation of metal – chalcogen clusters, the structures of which are dependent on the metal and the nature of the chalcogen moiety. One such example is the copper selenolate $[Cu_4(SePh)_4(dfbdp_)_2]$. Such luminescent molecular frameworks have emission energies that are dependent on the cluster composition and overall structure. The preparation, characterization and photophysical properties of several of these metal chalcogenolates will be presented.

Characterization and Electrocatalytic Performance of Amorphous Transition Metal Oxides

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Water electrolysis reaction has received renewed attention recently due to its potential to produce hydrogen gas in a greener fashion (with no CO_2 emission when hydroelectric or solar power is used). However, the slow kinetics of the oxygen evolution reaction (OER) and its rate limiting step acts as a barrier to utilize this reaction for mass hydrogen production. Designing an efficient catalyst for OER using transition metal oxides seems to be the viable solution. Previous work in Morin's group has shown good electrocatalytic activities of various binary and ternary spinel oxides containing Fe, Ni, Cu and Co. In this work, we have chosen five spinel oxides (namely $Cu_{0.9}Fe_{0.1}Co_2O_4$, $Ni_{0.9}Fe_{0.1}Co_2O_4$, $Cu_{0.5}Ni_{0.5}Co_2O_4$ $CuCo_2O_4$, Co_3O_4), and synthesized their amorphous analogues using a photochemical decomposition method to compare their properties. These materials have been characterized by X-ray diffraction, scanning electron microscopy and energy dispersive X-ray spectroscopy. Moreover, their electrocatalytic activity was investigated using cyclic voltammetry. The goal is to understand the relationship between the structure of the surface and its catalytic activity by comparing these results to that of their spinel counterparts. These results will be discussed in the context of the materials' composition, structure, and catalytic properties.

Surface Grafting of a Donor-Chromophore-Acceptor Assembly onto Zinc Oxide Nanowires for Alcohol Oxidation

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Dye sensitized photoelectrochemical cells (DS-PEC) have emerged as a potential candidate for solar energy to fuels conversion. Herein, we report a new copper(I)-based donor-chromophore-acceptor triad containing a triphenylamine electron donor and dipyrido[3,2-a:2',3'-c]phenazine electron acceptor as the photoactive component for DS-PECs. Excited

state energy levels of this new triad are carefully aligned for thermodynamically favorable electron transfer to give a long-living charge separated state upon light illumination. This triad is surface grafted onto zinc oxide nanowires grown onto a conducting glass to construct the photoanode of the DS-PEC. Photoelectrochemical studies reveal efficient electron transfer to the conduction band of the nanowires. Further, this DS-PEC is utilized in performing various oxidative processes such as alcohol oxidation, water oxidation, and tertiary amines illustrating its potential in solar energy conversion.

Studying energy transfer dynamics between Perovskite Nanocrystals and Coordination Compounds

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$CsPbBr_3$ perovskite nanocrystals, due do their tunable band gap in the visible region, low cost, and abundant surface anchoring sites, are promising candidates as photosensitizers in hybrid materials for solar energy conversion. Metal coordination complexes are highly synthetically tailorable materials with superior catalytic ability, excellent electron transfer and storage abilities, but often have a limited visible light response. This work aims to attach coordination compounds onto perovskite nanocrystals and understand the energy transfer dynamics between the two. $CsPbBr_3$ perovskite nanocrystals are synthesized using a hot injection method and $Ru(bpy)_3(PF_6)_2$ was chosen to be the model complex to be studied. The Ru-$CsPbBr_3$ composites were thoroughly studied via techniques including photoluminescence, quantum yield, FT-IR, UV-Vis spectroscopy, and emission lifetime measurements. This study could pave the way towards designing similarly coupled composites with superior catalytic activity towards solar fuel generation.

Structure-reactivity studies on hypervalent squarepyramidal dithieno[3,2-b:2',3'-d]phospholes

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Conjugated organophosphorus compounds are extensively investigated for their utility in organo-electronic devices. Dithienophospholes are one such popular scaffold of interest. In addition to their highly luminescent nature, they can effortlessly be modified for various applications by chemical or geometrical modification of the main scaffold or phosphorus center, respectively. In this contribution, geometrical modifications of the phosphorus center is achieved by generating hypervalent compounds by [4+1] cycloaddition of trivalent dithienophospholes with o-quinones. The synthesized pentacoordinate molecules adopt unexpected square pyramidal geometry, thus generating a Lewis acidic phosphorus center. Interestingly, the molecules are stabilized via supramolecular π-stacking interactions in the solid and solution states, but show intriguing reactivity related to that of Lewis acids in the presence of suitable polar substrates. The photophysical properties and unusual reactivity of these new species are the topic of this presentation.

A Structural, DFT and Experimental Investigation of the Ring Stability and Ring-Opening Polymerization Behaviour of Cyclic Thionylphosphazenes in the Presence of Lewis Acid Catalysts

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A series of cyclic thionylphosphazenes were prepared and density functional theory (DFT) calculations initiated to gain insight into their susceptibility to ambient ring-opening polymerization with Lewis acid catalysts (GaCl3, AlCl3). DFT analyses determined that PBE1PBE-GD3BJ provided the optimal calculated structures for 1, 5, 5' and 8. The gauge-independent atomic orbital (GIAO) method (M05-2X-GD3//PBE1PBE-GD3BJ) provided a good approximation for the 31P NMR resonances. Energy calculations indicate that thionylphosphazene phosphorus substitution promotes heterolytic cleavage of the thionyl S–Cl bond, as does adduct formation with GaCl3 or AlCl3, suggesting that 4 has potential for GaCl3-

catalyzed ROP reactions at ambient temperatures. The generation of thionylphosphazene cation from 1 with catalytic quantities of Lewis acids (10:1 GaCl3, AlCl3) initiates the ambient temperature ROP to poly(thionylphosphazene) (2) in a minimum amount of solvent. Polymerization/ depolymerization studies of 1 and 2 in solution was found to be fully reversible in the presence of GaCl3.

Exploiting exo and endo furan-maleimide Diels-Alder linkages for the functionalization of organoruthenium complexes

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Diels-Alder cycloadditions (DA) involving furans-maleimides are extensively used in organic chemistry and materials synthesis. The thermoreversibility of this reaction has been widely exploited for many years in organic and material synthetic chemistry using elevated temperatures. More recently, we and others have shown that retro Diels-Alder (rDA) reactions of endo adducts can take place at biologically-relevant temperatures, making DA-type linkages as a promising tool for the stimuli-responsive delivery of drugs/drug candidates functionalized with cell-targeting/penetrating agents. This field of research is still in its infancy and the potential of DA-containing metal-based drugs/drug candidates has so far only scarcely been examined. Given the promising advances of organoruthenium complexes in cancer therapy, our group is interested in exploring the possibility of exploiting DA linkages as a mean to modulate the biological properties of such complexes. This presentation will focus on synthetic strategies to afford cationic furan-containing half-sandwich Ru(h6-C6H6) complexes (bearing an N,N-donor ligand) with two maleimides of a different electronic nature via a DA-type linkage. Preliminary results on their relative potential to disassemble (undergo a rDA reaction) under biologically-relevant conditions will also be discussed. These research findings could contribute to the development/design of improved delivery systems involving ruthenium- or other metal-based drug candidates.

Tunable Nanofibers from Benzene-1,3,5- Tricarboxamide Supramolecular Assemblies

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Benzene 1,3,5 tricarboxamides (BTAs) are an important supramolecular building block as their functional diversity makes them suitable for a range of applications, from nanotechnology to biomedical applications. BTAs can self-assemble into helical stacks due to three-fold intermolecular H-bonding. The ability to control the length of supramolecular polymers is of great interest for practical applications such as in sensors or organic electronics. However, there have been very few reports of nanofibers of controlled length constructed from BTA molecules. Recently, we have functionalized BTA molecules with metal complexes to observe the effect of metal-metal interactions on the stacking of the molecules. It was observed that the BTA-metal complexes surprisingly, rapidly self-assemble into fibers of low polydispersity. An investigation of the factors that affect the length of the fibers was performed and the length of the nanofibers was easily tuned by modifying the self-assembly conditions. The mechanism and kinetics of supramolecular polymerization were characterized by transmission electron microscopy and dynamic light scattering. We believe that this approach can be expanded to other metals and facilitate the preparation of conducting BTA fibers for a range of applications.

Self-Replicating DNA Based Nanoassemblies

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DNA nanostructures and nanoassemblies are promising materials in diagnostics, drug delivery, electronics, energy production, and other areas of materials science because of their easy synthesis, superb biocompatibility, and easy functionalization. Although scientists have developed DNA mediated nanoparticle machines and nanoassemblies that can

do specific tasks, these hybrid materials cannot self-replicate. Therefore an outstanding goal is to make self-replicating nanoassemblies. The amplification of these self-assembled nanosystems can be achieved by introducing turnover into DNA templated reactions with the hybrid nanomaterials. The Gibbs group has developed lesion induced DNA amplification (LIDA) strategy to achieve turnover in an isothermal DNA self-replication reaction utilizing ligase enzyme and exploiting the sensitivity of the DNA duplex to the presence of the destabilizing lesion. My research project aims to demonstrate the self-replication of DNA-modified gold nanoparticle (AuNP) shape assemblies. DNA will contribute toward the organization of the AuNPs into well-defined shapes with desired spacing. LIDA will allow the self-replication of these nanoassemblies.

Does exposure to microplastics during pregnancy impact fetal and placental development?

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The worldwide use of plastics has resulted in a vast accumulation of microplastics in the air, soil and water. Through all of these environments microplastics can find their way to enter animals and humans and accumulate in tissues. The detrimental effects of microplastics on marine life have been investigated extensively; however, the impact of microplastics on human health remain unknown. One significant knowledge gap is the impact of microplastics during pregnancy.

Here, we exposed pregnant CD-1 mice to different concentrations (1000, 10, 0.1, and 0 ug/L) of 5 micrometer polystyrene in drinking water throughout gestation. The use of experimental mice allows us to establish causal relationships between environmental exposure and pregnancy outcomes. Pregnant mice were sacrificed at 17.5 days of gestation (full term is 18.5 days). Fetal weights, placental weights and umbilical cord lengths were recorded, and placental tissues were collected to study the metabolite profiles using high-resolution magic angle spinning magnetic resonance spectroscopy.

With the completion of this project, we have established that maternal exposure to microplastics impacts fetal growth and placental metabolic pathways. This information is critical to establishing guidelines to limit exposure and to prevent adverse pregnancy outcomes that result from microplastics.

Exploring the Bacterial Preference in Degradation of Terrestrial and Marine Organic Matter of St. Lawrence Estuary by Stable Carbon Isotope Signature

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Estuaries, as important biogeochemical sites with diverse ecosystem and a strong salinity gradient due to the mixing of fresh river water and salty ocean water, are great reservoirs of organic matter (OM). Stable carbon isotope ratios ($\partial^{13}C$) of either bulk OM or specific organic compounds in these zones gives detailed information about a wide range of processes such as carbon cycling, tracing of biomarkers, bacterial activity, etc. The $\partial^{13}C$ signature of marine organic carbon (MOC) in sediments is about -22 ‰, while that of terrestrial organic carbon (TOC) is about -28 ‰, leading to gradual changes in the signature of sedimentary OC along the terrestrial-marine continuum in estuaries. Because of its biochemical composition, marine OM is generally considered more easily biodegradable than terrestrial OM. It is thus expected that this preference would be reflected in the $\partial^{13}C$ signature of biomarkers that are specific to heterotrophic bacteria (branched iso- and anteiso-C15:0 and C17:0 fatty acids), with compound-specific signatures being more enriched compared to the expected values if the biolability of both terrestrial and marine OM was identical. However, previous work has shown that the $\partial^{13}C$ signatures of bacterial fatty acids suggested that bacteria displayed no preference towards terrestrial or marine OM.

Mass spectrometry identifies sialoglycans as attachment factors of SARS-CoV-2

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Spike (S) glycoprotein of SARS-CoV-2, which is responsible for binding to the host receptor angiotensin-converting enzyme 2 (ACE2), mediates viral entry. There is emerging evidence that host glycans serve as attachment factors that enhance cell binding and infection. To identify human glycans recognized by SARS-CoV-2, we employed catch-and-release electrospray ionization mass spectrometry (CaR-ESI-MS) assay. S protein and its receptor binding domain (RBD) were screened against a defined library of 139 glycans, most of which are present in mammalian cells. Notably, both S protein and RBD recognize sialic acid-containing glycans (sialoglycans), with preference for monosialylated ganglioside oligosaccharides with dissociation constants Kd of 100-200 μM. These affinities are similar to heparan sulfates oligosaccharides, negatively charged glycans proposed as SARS-CoV-2 S protein co-receptors. Many other classes of neutral and acidic human glycans are recognized by RBD, albeit weakly. The results of competitive binding measurements suggest the presence of multiple binding sites, with distinct preference of acidic and neutral glycans. RBD also binds monosialylated gangliosides embedded in an artificial lipid bilayer. Screening of natural N-glycans libraries derived from lung and intestinal tissues against RBD revealed monosialylated monoantennary N-glycans as preferred structure. Overall, acidic sialoglycans, particularly glycolipids, are suggested to serve as SARS-CoV-2 attachment factors.

High-performance Electrocatalysts for Metal-Air Batteries

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The search for non-precious electrocatalysts for air-operated energy systems is emerging, since metal-air batteries are important power sources due to their high energy density and low cost. These features of metal-air battery give them five stars! In order to fully utilize these energy systems, electrocatalysts with improved kinetics towards electrochemical oxygen reduction reaction (ORR) and oxygen evolution reaction (OER) process are required. The first generation of ORR/OER electrocatalysts operated on precious metals such as platinum. However, the sluggishness of electrochemical reactions, economical issues and limited resources of noble metals motivates for development of new high-performance, environmentally benign, and cheaper catalyst that can react with oxygen. Metal-organic frameworks (MOFs) are fascinating motifs that have been extensively investigated and proposed in many applications that require a well-defined porosity and expanded surface area. The MOF-derived electrocatalysts benefit from these features of MOF, resulting in air-breathing cathodes with acceptable electrochemical activity that are made of abundant elements like carbon, thus allowing for replacement of expensive cathodes in metal-air energy systems.

Evolution of Used Fuel Container Corrosion from Oxic to Anoxic Conditions

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Continuing use of nuclear power strongly depends on the proper management of highly radioactive nuclear waste. The internationally accepted plan for nuclear fuel waste disposal is to bury sealed spent nuclear fuels in the corrosion-resistant containers surrounded by bentonite buffer blocks, in a deep geological repository. The proposed container in Canada is a copper-coated carbon steel vessel. Once the Cu-coated container is emplaced in the repository, it will be exposed to conditions which evolve from oxic and warm to anoxic and cool over time. After sealing the repository, oxygen introduced during the initial construction phase will be consumed by reaction with minerals, microbial activity, as well as reaction with the copper coating. As a result, it's expected the surface of container will be covered by corrosion products including cuprite (Cu_2O), tenorite (CuO) and other types of oxide in the presence of various anions in the groundwater chemistry. Once anoxic condition is established, the only available oxidant is dissolved sulfide that could diffuse through the bentonite buffer box, reaches the container, and converts the Cu oxide to Cu sulfide.

The conversion of copper oxides to sulfide and its effect on corrosion behavior of copper is the main goal of this work.

Metabolomic analysis of human urine and plasma by liquid chromatography-high resolution mass spectrometry

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Metabolomics aims at quantifying metabolic changes from a biological sample by measuring small molecule metabolites. Urine and plasma are commonly used in metabolomics due to their wide range of metabolites and their accessibility. An unusual variation of these metabolites can predict changes occurring from dietary changes, environmental contaminants or pharmaceuticals, as well as serve as potential biomarkers of certain metabolic diseases.

The aim of this study was to develop an LC-MS/MS method to cover the wide range of metabolites present in urine and plasma samples. For this, we compared four chromatographic columns and different sample extraction procedures, including protein precipitation, solid-phase extraction, dilution and the Bligh-Dyer method. We also determined the inter-day variability between individuals on the urine metabolomic profile, and the effect of normalization for creatinine concentrations in urine samples.

Two complementary separations have been chosen to cover a large number of urinary metabolites. For sample preparation, a dilution of urine, with creatinine normalization, gave the best results while a protein precipitation in plasma samples allows a better extraction of plasma metabolites.

ABSTRACTS // BIOCHEMISTRY & MOLECULAR BIOLOGY ORAL PRESENTATIONS

Controlling the evolution of antimicrobial resistance with collateral sensitivity loops

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With rapid emergence of bacterial antibiotic resistance, novel antimicrobial strategies to combat resistance are required. One such strategy could be to exploit the increased susceptibility bacteria exhibit to some antibiotics as they become resistant to others, a phenomenon known as collateral sensitivity. In principle, these collateral sensitivities can be chained together, such that bacteria will always remain susceptible to at least one antibiotic. To illustrate this, consider a bacterial population undergoing sequential treatment with drugs A, B and C. When resistance to drug A evolves, treatment will be switched to drug B, to which the drug A-resistant population exhibits collateral sensitivity. As resistance to B emerges, the next drug C will be applied to which drug B-resistant population exhibits collateral sensitivity. Drug C will be chosen such that it reinstates susceptibility to drug A. To identify potential antibiotic sets I will utilize the high throughput capability of the Soft Agar Gradient Evolution (SAGE) system developed in our lab, sequentially developing antibiotic resistance and assessing the resulting collateral sensitivity. With one or more sets of antibiotics identified that consistently lead to collateral sensitivity loops, this work may lead to a strategy to control antimicrobial resistance evolution.

Dark Dynamic Therapy: Photosensitization using a Dioxetane-Erythrosin B Conjugate

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Photodynamic therapy is a clinically approved cancer treatment that involves light excitation of a photosensitizer to produce reactive oxygen species (e.g., singlet oxygen). Although singlet oxygen is an effective cytotoxic agent, the requirement of light for its production is limiting due to the poor light penetration depth in tissues and the light delivery systems available. Thus, developing a photosensitizer that can be excited without an external light source (i.e., dark dynamically) is desirable. To this regard, we have designed a dark dynamic probe based on Schaap's chemiluminescent scaffold containing an adamantylidene-dioxetane moiety. We demonstrate that by attaching the photosensitizer, Erythrosin B, the resulting dioxetane breakdown leads to energy transfer from the chemiluminescent scaffold to Erythrosin B, followed by singlet oxygen production that can induce cytotoxicity at low micromolar concentrations. My presentation will discuss the concept of dark dynamic therapy using a cell permeable, small molecule capable of photosensitization without light.

Investigating the effects of microRNA expression on the kidney of the thirteen-lined ground squirrel, Ictidomys tridecemlineatus, during torpor

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During the hibernation season, the thirteen-lined ground squirrel undergoes cyclical torpor and arousal periods. The decrease and restoration of metabolic rate and oxygen delivery during torpor and arousal, respectively, may cause reperfusion-ischemia injury in the kidneys. In order to maintain the structural integrity of the kidneys necessary for renal function resumption during arousal, the thirteen-lined ground squirrel has developed adaptive methods to prevent and repair kidney injury.

In this present study, computational methods were used to clean and analyze sequenced kidney RNA samples. Significantly differentially expressed microRNAs and enriched gene sets were also determined. From the gene set analysis, the results showed an increase in ubiquitin-related processes and p53 signaling pathways which suggested the occurrence of kidney damage during torpor. There was also an observed increase in cell cycle processes and the anchoring junction cellular compartment which may lend to the prevention of kidney injury. From the differentially expressed microRNAs, miR-27a, miR-129, miR-let-7b, miR-let-7c and miR-let-7i were found to be significantly upregulated and to contribute to the prevention of kidney lesions. These biochemical adaptations may allow the thirteen-lined ground squirrel to maintain kidney structure and function during hibernation.

Towards Structure-Guided Design of Aminoglycoside Phosphotransferase Inhibitors

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Aminoglycosides are a broad-spectrum class of antibiotics used to treat serious gram-negative and gram-positive bacterial infections. However, widespread resistance has led to a decrease in aminoglycoside clinical use. This resistance can be established through aminoglycoside-modifying enzymes such as APH(2'')-Ia, which inactivates aminoglycosides through phosphorylation of hydroxyl groups. One strategy to circumvent aminoglycoside resistance is by inhibiting APH's activity. The production of inhibitors for this class of enzymes is exceedingly challenging, as APHs are structurally similar to eukaryotic protein kinases. We hypothesize that through fragment-based drug-discovery techniques, differences between human and bacterial homologues can be exploited to generate inhibitors specific to APHs. Through saturation transfer difference and waterLOGSY nuclear magnetic resonance experiments, we have screened and identified fragment molecules which bind to APH(2'')-Ia. X-ray crystallography will be used to determine the position and orientation of

fragment binding. Based on structural data, successful fragments can be further expanded to form a drug candidate capable of binding to APH(2'')-Ia with high affinity and specificity without disrupting the essential functions of mammalian protein kinases. Such an inhibitor could allow for continued use of aminoglycoside antibiotics in the treatment of otherwise resistant bacterial infections.

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

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

TRAPPC10 variants are associated with neurodevelopmental disorder and microcephaly in humans

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Background The highly evolutionarily conserved transport protein particle (TRAPP) complexes (TRAPP II and III) perform fundamental roles in subcellular trafficking pathways. Defects in this process are associated with various human disorders. Recently, a homozygous missense p.(Pro929Leu) variant in TRAPPC10, a component of the TRAPP II complex, was reported in two affected adult male siblings with microcephaly and severe neurodevelopmental disorder.

Methods We undertook whole exome sequencing on a large interlinking multi-nuclear family, to identify the likely cause of a severe neurodevelopmental disorder in eight affected siblings. We performed functional studies to assess the effect of the identified TRAPPC10 variant on membrane trafficking and Ciliogenesis.

Results A homozygous deleterious frameshift variant, p.(Gly1131Valfs*19) in TRAPPC10 was identified in the affected siblings. Using a yeast two-hybrid assay we demonstrate that the two TRAPPC10 variants have reduced interaction with its adaptor protein TRAPPC2L. Size exclusion chromatography studies of patient lymphoblastoid cells suggested that the variant p.(Gly1131Valfs*19) affects the assembly of TRAPP complexes due to absence of TRAPPC10 alongside an absence of TRAPPC9, another key TRAPP II complex component associated with a clinically overlapping neurodevelopmental disorder. The TRAPPC9/10 reduction phenotype was recapitulated in TRAPPC10-/- knockout cells, which also revealed a membrane trafficking and ciliogenesis defect.

Synthesis of Carbamoyl Fluorides with a Difluorophosgene Surrogate

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While carbamoyl chlorides have received much attention from the synthetic community as a molecular building block, the related carbamoyl fluoride has only emerged as an alternative in the last three years. These fluorine-containing electrophiles have demonstrated unique reactivity compared to the chloride, and their limited use can be attributed to the lack of practical preparations available. Several methods exist, however most require non-commodity starting materials and the use of volatile, dangerous, or expensive reagents. Using (triphenylphosphonio)difluoroacetate (PDFA) as an air and moisture-stable source of difluorocarbene and pyridine N-oxides as an oxidant, we have developed an efficient, mild synthesis of carbamoyl fluorides. This method demonstrates a broad scope, accessing carbamoyl fluorides containing biologically relevant heterocycles, amino acid fragments and functional groups that would typically react with difluorocarbene. Control experiments, in-situ NMR analysis and initial rates kinetics have provided evidence of an unusual reaction mechanism that differs greatly from known carbamoyl fluoride syntheses and difluorocarbene oxidation systems.

Copper-Promoted N-Arylation of the Imidazole Side Chain of Protected Histidine using Triarylbismuth Reagents

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UQÀM

With more than 950 peptides having drug-like properties, peptides stand out in new class of clinical therapeutics. Indeed, because of their high specificity, biocompatibility and biodegradability, they rapidly became a point of interest in drug development. However, peptide chemoselective modifications are known to be notoriously difficult. Developing new amino acid functionalization method is thus essential to bring out efficient tools towards peptide modification. Bismuth is a heavy metal with low toxicity. Organobismuth compounds can be used to transfer organic groups to a variety of nitrogen, oxygen and carbon nucleophiles. Over the last decade, our group developed a series of copper-catalyzed methods to realize coupling reactions between aryl bismuth species and heteroatoms such N, O and S. In this presentation, I will share our results on the development of the N-arylation of the side chain of histidine and small histidine-containing peptide catalyzed by copper cross-coupling and using triarylbismuthines. Our investigation into the unexpected histidine-directed backbone peptide arylation reaction will also be presented.

Diverse binding modes of [3+3] Schiff-base macrocycles with ammonium guests

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Within the last few decades, chemists have designed an array of macrocyclic compounds that bind strongly and selectively to form discrete supramolecular structures with a chosen guest. Herein we present the opposite, a promiscuous [3+3] macrocyclic host 1 which binds to diaryl- and dialkyl- ammonium guests with a range of binding modes and tautomeric forms. We studied the host-guest chemistry with dibenzyl ammonium (DBA+), dipropyl ammonium (DPA+), and dixylyl ammonium (DXA+) all of which showed different responses owing to their varying electronic and steric properties (Figure 1). We then showed that DBA+ could act as an effective template for the formation of 1 from starting materials.

Nickel-Catalyzed Deoxygenation of Diverse C-O Bond-Bearing Groups: The Hunt for Potential Intermediates

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While accessing complex molecules is central to the pursuit of organic synthesis, there is also value in the discovery of reactions that decrease complexity. For instance, methods for late-stage defunctionalization can be applied towards the reduction of biomass-derived feedstocks – a transformation that exists as paramount in the push towards a bio-friendly chemical industry – as well as towards the removal of protecting or directing groups for use in synthesis. Recently within our group, a nickel-catalyzed system has been developed that permits the exhaustive deoxygenation of C(sp3)-O bonds in alcohols, ethers and epoxides; unsaturated species including aldehydes, ketones and esters are also deoxygenated via the initial formation of a silylated alcohol intermediate. Mechanistically, nickel-catalyzed C-O bond activation has been demonstrated to occur via non-obvious, complex substrate dependent mechanisms. By combining a kinetic analysis with a series of control experiments performed on substrates prone to rearrangement, we demonstrate that our reaction proceeds through a complex mechanism involving the presence of a key radical-organonickel hybrid intermediate.

Stimuli Responsive Triggered Self-immolative Pseudopeptides

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With a 5-year survival rate under 7% and 10-year survival rate under 1%, glioblastoma multiforme (GBM) is the most common type of malignant brain tumour and it is almost always lethal.1 However, it is extremely difficult to treat GBM and surgical removal does not clear the tumour completely. GBM responds to anticancer medicines, however, there exist two great challenges faced by chemotherapeutic treatments: the issue of getting the medication across the blood brain barrier (BBB) and a character of GBM called polymorphism which means it exists in many different forms, making it hard to target as there are many different possible mutations. Self-Immolative NanoCapsule (SINC) is a class of novel drug delivery molecule that can deliver the medication across the blood brain barrier. We wish to discuss our progress towards third generation SIP systems that use a linear biodegradable, non toxic and potentially amphiphilic backbone, derived from amino acid building blocks. The potential for differential functionalization makes the resulting SIPs useful as biocompatible traceless drug-delivery capsules and as the basis for biomedical device development.

Conglomerate Crystallization Under the Influence of the Chirality Induced Spin Selectivity (CISS) Effect

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Electron transmission through chiral molecules is spin-dependant. Central to the research on the influence of the Chiral Induced Spin Selectivity (CISS) effect on chiral recognition and conglomerate crystallization is the use of a ferromagnetic surface, comprised of a gold coated nickel layer, where the orientation of the electron spin at the nickel layer can be controlled by simply changing the orientation of a permanent magnet positioned underneath the substrate. Chiral molecules can become momentarily spin-polarized upon charge polarization. By charge polarizing a chiral molecule with zero spin, an induced dipole is formed in the molecule. Each enantiomer of a chiral molecule can interact differently with a spin polarized surface. Herein, crystals that form chiral conglomerates were grown on spin filter surfaces to explore spin dependant resolution. The crystallization of racemic mixtures of asparagine and glutamic acidHCl were investigated, along with sodium chlorate and benzil, achiral molecules that also crystallizes as conglomerates. Chiral crystals were formed on the ferromagnetic substrate from supersaturated solution or by sublimation. The crystals were collected, and the enantiomeric excess of the crystals was determined using solution or solid-state circular dichroism spectroscopy. CISS effect allows the enantiomers to be separated from each other simultaneously.

Chemically tuning covalent antibody recruiting molecules to modulate immune recognition and response: An application of sulfonyl fluoride exchange chemistry

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In the field of immunotherapy, small molecule strategies have driven significant insight into the mechanisms of immune recognition. To investigate the binding dynamics of the immune response *in vitro*, the Rullo lab has developed dual-binding compounds known as covalent immune recruiters (CIRs). CIRs are synthesized with three functional domains: an antibody-binding domain (ABD), an antibody labelling domain and a tumor binding domain (TBD). Proximal to the ABD, the ALD contains an electrophilic group which is attacked by a nucleophilic amino acid residue on the target antibody. In previous designs, CIRs were developed with an acyl-imidazole ALD which successfully probed anti-DNP IgG in human serum. To expand the scope of CIR technology, a new type of click chemistry, sulfur fluoride exchange (SuFEx), will be explored in the next generation of CIRs. Sulfur fluorides have been broadly used in academic and industrial application to label numerous amino acids including lysine, tyrosine, serine, cysteine, histidine, and threonine. SuFEx chemistry is expected to improve the hydrolytic stability, binding kinetics and selectivity of current CIR designs. Through this platform, CIR technology will contribute design principles and mechanistic insight into antibody dependent immune recognition of cancer.

A Scalable Desymmetrization of Poly(-ynes) By A Copper (II) Mediated Synthesis of 3,5- Disubstituted Isoxazoles Via 1,3-Dipolar Cycloadditions of Nitrile Oxides and Terminal Alkynes Under Planetary Ball-Milling Conditions

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Desymmetrization of poly(-ynes) *via* 1,3-dipolar cycloadditions of nitrile oxides and terminal alkynes to form 3,5-disubstituted isoxazoles is a current challenge in organic synthesis as reactions require the use of protecting groups, excess amount of one of the substrates, and careful temperature control to desymmetrize the molecules efficiently. Thus, these reactions suffer from poor atom economy, poor selectivity (formation of the polyisoxazoles over the monoisoxazole adduct), and higher hazardous waste production. As an alternative, mechanochemistry has emerged as a sustainable technique used to efficiently desymmetrize symmetric organic precursors into complex organic molecules with a lower environmental impact than solution-based methodologies. Herein, we describe a scalable desymmetrization of symmetric poly(-ynes) by a copper (II)-mediated synthesis of 3,5-disubstituted isoxazoles *via* 1,3-dipolar cycloaddition under planetary ball-milling conditions that were applied to a wide range of poly(-ynes) in low to excellent yields, in short reaction times, and with a lower environmental impact than solution-based methodologies.

Guanidine Derivatives and their Application Towards Pancreatic Cancer Treatment

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Pancreatic cancer can be considered as one of the most uncured cancers of the 21st century. Metformin, a biguanide antidiabetic drug, has shown interesting anti-cancerous properties towards pancreatic cancer in vitro and in mice. Its biological activity resides in the inhibition of the mitochondrial respiratory chain, leading to cellular death. However, the high hydrophilicity of biguanides moieties prevents their diffusion through phospholipid bilayers. We present and discuss our efforts to design more amphiphilic guanidine derivatives able to cross the cellular and mitochondrial membrane, their biological activities and application in cancer treatment.

Our strategy is then to use guanidine analogs such as iminoguanidines and cyanoguanidines, as they have proven to be good pharmacophores for the treatment of other types of cancer and possess anionophore properties. Thus, our approach is to combine hydrophobic scaffolds able to penetrate phospholipid membranes with these groups in order to increase their uptake inside the cell. In this way, we hope to develop more efficient anticancer drugs, able not only to interfere

with the mitochondrial respiratory chain, but also able to modify the homeostatic regulation of ionic gradients in mitochondria.

Using molecular design to study the self-assembly of multicomponent low molecular weight gelators
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Supramolecular gels composed of low molecular weight gelators (LMWGs) are a class of physical gels where one or multiple components self-assemble through non-covalent interactions. There are several ways in which multicomponent LMWGs may self-assemble: 1) co-assembly, where all components randomly assemble into fibers; 2) social self-sorting, where one component has an affinity to the second component, creating alternating fibers; 3) narcissistic self-sorting, where each component only interacts with itself. The effect of molecular structure on the self-assembly is still not well understood, but may lead to principles to produce gels with pre-designed properties. We investigated the effect of molecular structure on self-assembly in a library of amino-acid based LMWGs that differ in their headgroup and the length of the alkyl chain, leading to variation in hydrophobicity and intermolecular interactions. We analyzed the multicomponent gels using differential scanning calorimetry, variable-temperature nuclear magnetic resonance spectroscopy and small angle X-ray scattering to determine the packing preference. Furthermore, we performed statistical analysis to investigate the role of hydrophobicity and chain length on the overall pathway of self-assembly for these multicomponent systems. Understanding the nuances of the self-assembly processes, allows one to predict the behavior of gelators in multicomponent systems.

Development Towards a Lewis Acid Catalyzed Intramolecular Acylfluorination Method
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Acyl fluorides are versatile intermediates in organic synthesis due to their superior stability and distinct reactivity when compared to other acyl halides. While many examples of their use as cross-coupling partners exist in the literature, until recently few reactions utilized them in fluorinative transformations. Acyl fluorides are readily available from cheap nucleophilic fluoride sources and upon fluoride abstraction can form a highly electrophilic acylium ion, an ideal intermediate for reaction with π-nucleophiles. Efforts towards the development of a Lewis acid (LA) catalyzed carbofluorination reaction of acyl fluorides and alkynes will be presented. Initial catalyst screenings have identified a set of boron and carbon-based Lewis acids suitable for the proposed transformation with substrate controlled E/Z selectivity of the resulting monofluorinated alkene. Further mechanistic studies have provided evidence for divergent mechanistic pathways depending on the class of LA used. Additional investigations into substrate scope revealed that alkynes with aromatic substituents tolerated the reaction with greater success than aliphatic substituents.

Intramolecular Nickel- and Palladium-Catalyzed Ring-Opening Reactions of Oxabicyclic Alkenes with C1-Tethered Aryl Halides
A. Pounder[*], S. Koh, L. D. Chen, W. Tam
University of Guelph

Oxabicyclic alkenes, including oxabenzonorbornadienes and its derivatives, are a class of 1,4-epoxides which can be readily activated by transition metal complexes with great facial selectivity. Of particular interest are nucleophilic ring-opening reactions of oxabicyclic alkenes, as they provide access to a broad family of synthons bearing multiple stereocenters in a single step. Previously, the Tam group, as well as others, have reported intermolecular modes of reactivity using a plethora of transition-metal catalysts. Herein, we report the first examples of intramolecular nickel- and palladium-catalyzed ring-opening reactions of oxabicyclic alkenes to form tetracyclic frameworks. Depending on the reaction conditions used, both the 1,2-dihydronaphthalen-1-ol and dehydrated naphthalene products were synthesized in excellent yield and selectivity.

Predictable color-tuning in multicomponent photoluminescence systems & its application
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Molecular photoluminescence is the basis for multiple analytical techniques and lighting/display technologies. For example, the design of white light-emitting organic materials has received much attention owing to the potential for low-cost lighting and displays. It is commonly accepted that white light emission can be produced by mixing multiple simultaneously emitting molecules, however, an approach to rationally mix different colored emitters to achieve a desired chromaticity had not been reported. In this work, we were able to identify a simple formula to predict the color resulting from mixtures of two and three simultaneously emitting organic molecules. By mitigating the potential for energy transfer, the emission chromaticity is shown to be controlled by adjusting 1) the ratios of each component and 2) the excitation wavelength used to excite the system. This strategy was then exploited to target highly desirable white light emission (CIE = 0.33, 0.33) using a predetermined combination of perylene (blue), coumarin 6 (green), and Nile Red (red). In addition to applications to materials, this relatively simple approach may be further used to realize novel PL-based sensing systems and anticounterfeit technologies.

An Electrochemical Approach to Palladium-Catalyzed Carbonylative Coupling Reactions
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Carbonyl-containing compounds are ubiquitous in nature and of great importance to pharmaceutical and material sciences. Classical synthetic routes, often through electrophilic agents such as acyl chlorides, involve using high-energy reactive starting materials or reagents of poor atom economy. Transition-metal catalyzed reactions, in particular carbonylation, offers one of the most efficient and atom-economical approaches to carbonyl-containing compounds from simple organic building blocks. However, traditional thermal carbonylations face challenges from oxidative addition and reductive elimination, two steps critical for catalytic turnover, as they present opposite chemical requirements for the catalyst and thus demand careful design. Herein, we report the development of a redox-neutral electrochemical carbonylative coupling reaction. The use of electricity drives the catalytic cycle and allows acyl chloride to build up in solution, thus enabling a broad scope of nucleophiles to be used for the facile assembly of diverse molecular structures.

QSAR Model of EPAC1-Selective Modulators

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Exchange proteins directly activated by cAMP (EPAC) are guanine nucleotide exchange factors for the small GTPases, Rap1 and Rap2. They regulate several physiological functions and mitigation of their activity has been suggested as a possible treatment for multiple diseases such as cardiomyopathy, diabetes, chronic pain, and cancer. Several EPAC-specific modulators have been developed, however, studies that quantify their structure-activity relationships are still lacking. This study, therefore, proposes a quantitative structure-activity relationship (QSAR) model for a series of EPAC1-specific compounds. The model demonstrates high reproducibility and predictivity and its predictive ability was tested against a series of compounds originally unknown to the model. The compound with the highest predicted affinity was validated experimentally through fluorescence-based competition assays as well as NMR experiments. The model can, therefore, serve as a virtual screening tool for promising candidates to design EPAC1-selective drugs more effectively.

Computational Modelling of Prebiotic Autocatalytic Chemical Reaction Networks

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Complex chemical reaction networks can grow exponentially in terms of the chemical diversity they can generate. It is unknown whether such networks easily discover or shuttle fluxes through autocatalytic sub-networks. We aim to provide a map for experimental chemists studying complex organic reactions through an automated rule-based reaction generation to simulate the reaction network generated during the alkaline hydrolysis of glucose, which is a well-studied reaction providing ample data for ground-truthing. We applied graph transformation rules based on well-documented reaction mechanisms and used isomorphism tests to match the output molecular structures to experimentally reported structures as a test of the completeness of our methods. The monoisotopic exact masses of the molecules in the computed reaction network product set were calculated and used to match peaks identified in high-resolution FT-ICR-MS data of the same reaction. The reaction network was further assessed for the existence of potentially autocatalytic loops. This was done by loading the network topology (nodes being compounds and edges being reactions) into a graph database where pattern matching queries could be executed to search for patterns of interest. This work demonstrates some efficient methods for finding reaction pathways and autocatalysis in insilico modeled reaction networks.

Mechanism of Urea Oxidation on β-Ni(OH)$_2$ from First-Principles Simulations

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Urea-enriched water is a waste by-product in the industrial production and application of urea, with most urea produced going directly towards making nitrogen-based fertilizers. While current urea removal methods can sustainably treat contaminated water, they fail to extract the energy released in the destruction of the chemical bonds in urea. The electrochemical urea oxidation reaction (UOR) on nickel hydroxide-based electrocatalysts is a sustainable method to treat urea-enriched water that enables the capture of energy released during the oxidation of urea. Currently, we do not have a detailed atomic description of the different mechanistic pathways of UOR, and this knowledge would help improve electrocatalyst performance. Herein, we present density functional theory (DFT) calculations to determine the

thermodynamically most favourable reaction pathway by considering multiple different intermediates and adsorption sites for each reaction step on β-$Ni(OH)_2$. The computational hydrogen electrode (CHE) method is utilized in our model to fully capture the influence of the applied electrochemical potential and understand which pathway is thermodynamically most favourable under experimental conditions. The work presented here builds towards developing a more complete atomic-scale understanding of UOR at the surface of $Ni(OH)_2$-type electrocatalysts, which could aid experimental efforts in optimizing catalyst materials for this reaction.

ABSTRACTS // NANOCHEMISTRY ORAL PRESENTATIONS

Highly Organized Arrays of Gold Nanorings Assembled on Tobacco Mosaic Virus Coat Protein

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Bottom-up fabrication of precisely organized nanomaterials is a major challenge in materials science. Biological scaffolds show great promise as economical, monodisperse, programmable templates for synthesis of nanomaterials. Here we report the synthesis and characterization of highly organized arrays of gold nanoparticle (AuNP) rings assembled on a hexahistidine-tagged tobacco mosaic virus coat protein (6H-TMV-cp) template.

Near neutral pH, 6H-TMV-cp self-assembles into small disk-shaped particles. The His-tag is exposed on the edge of the disks. The disks are known to self-assemble into 2D hexagonally-packed sheets via His-His interactions. Here, we report two new nanostructures: cubically-packed sheets, and nanotubes from rolled up hexagonally-packed sheets.

The His-tag also interacts strongly with AuNPs to form rings of AuNPs around the disks. These AuNP rings are interesting because the plasmon bands of individual nanoparticles can couple together, leading to changes in the plasmonic effect within the radius of the ring.

Characterization of the nanoring structures by transmission electron microscopy, small angle X-ray scattering, UV-vis spectroscopy, and dark field optical microscopy is underway to investigate both the physical structure and the plasmonic behaviour of the systems. Extended structures of well-organized plasmonic nanorings have many potential applications, including as sensors, metamaterial superlenses, and waveguides.

Plant-derived phytoglycogen as a nanocarrier for the delivery of antimicrobial peptides

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Antimicrobial peptides, such as GL13K, have a high binding selectivity towards bacterial membranes, while not affecting healthy mammalian cells at therapeutic concentrations. However, the systemic delivery of these peptides can be challenging since they are susceptible to enzymatic hydrolysis, rapid elimination, and poor cellular uptake. A protective nanocarrier is thus proposed to prevent premature degradation. We investigated the potential to employ biodegradable phytoglycogen nanoparticles as carriers for GL13K. Both the native (quasi-neutral) and carboxymethylated (anionic) phytoglycogen were evaluated for their loading capacity, release characteristics, and antimicrobial activity. We show that the anionic nanophytoglycogen has a greater loading of the cationic antimicrobial peptide and exhibits slow-release characteristics. Isotope exchange measurements are consistent with the antimicrobial peptide being entrapped in the dendrimer pores, which should provide the necessary protection for delivery.

Discerning the bonding in polyaniline-chitosan composites

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A survey of various preparations of polyaniline (PANI)-biopolymer composites reveal that the nature of the bonding between PANI and chitosan (CHT) is not fully resolved. This study aims to discern the role of (non)covalent bonding in binary PANI/CHT composites prepared by three synthetic routes: *in situ* polymerization of aniline with CHT; self-assembly of PANI and CHT; physical blending of PANI and CHT. Various characterization methods were employed: powder X-ray diffraction, spectroscopy, thermal gravimetry analysis. Swelling tests provided absorption-spectral correlations, and dye adsorption revealed accessible adsorption sites. Results show that covalent grafting and H-bonding for PANI/CHT (*in situ* polymerized) composites. Bonding in self-assembled samples resembled that for physical blends, where H-bonding was shown via complementary methods. Swelling tests revealed *in situ* polymerization yielded the lowest water swelling, in line with the role of (non)covalent bonding from spectral results. Dye adsorption results revealed unique dye uptake for *in situ* polymerized composites. The highest dye uptake was obtained for PANI/CHT 50/50 system, where the Sips and Dubinin-Astakhov adsorption models describe results for the composites. *In situ* polymerization method yield covalent grafting of PANI onto CHT with partial hydrogen bonding, whereas composites prepared by self-assembly and blending favour noncovalent PANI-CHT interactions.

Size-controlled synthesis of bioinspired polyserotonin nanoparticles with free-radical scavenging property

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Polyserotonin-based nanoparticles are a new class of bioinspired nanomaterial with recently demonstrated therapeutic potential for future clinical applications. It is therefore important to establish a robust and rapid method of synthesizing polyserotonin nanoparticles (PSeNP) in the size range ideal for *in vivo* utilization. Since the formation of PSeNP is based-catalyzed, there we report the influence of solution pH, in the presence of different base systems, on the kinetics of PSeNP formation and physico-chemical properties of the resulting nanoparticles. We show that the rate of formation and the size of PSeNP depend on both the nature of the base and the initial pH of the reaction. We have also improved the kinetics of particle formation by performing the synthesis at an elevated temperature (60°C), leading to a dramatic reduction in synthesis time from days to hours. This presents a significant advance in the efficiency of PSeNP synthesis and provides a facile approach in tuning the size of nanoparticles to suit various applications. Furthermore, we show that similar to serotonin, PSeNP also exhibits free-radical scavenging property. Our results demonstrate that PSeNP has the potential to become a key player in the advancement of nanotehcnoogy-mediated antioxidative therapy.

Development of Multimodal Imaging Probes Using Carbon Dots

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Molecular imaging techniques have a significant role to monitor human health. However, these techniques possess some limitations. In this context, the design of probes that can be suitable for multiple molecular imaging techniques has been proposed as a new approach to address the issue. More specifically, carbon dots (CDs) have attracted significance in the medical field because of their biocompatibility, an important characteristic for clinical applications. This class of nanoparticles has demonstrated to improve the signals and diagnose diseases even at early stages. Herein, a dual-modal system based on carbon nanomaterials functionalized with a transition metal ion, Mn^{2+}, is presented. The intrinsic fluorescent properties of the carbon dots, attributed to the functional groups on their surface, makes them suitable as fluorescence imaging probes while the coupling of metals using a chelating agent, cyclic diethylenetriaminepentaacetic acid anhydride (cDTPAA), and a cross-linker, (1-ethyl-3-(3-dimethylaminopropyl) carbodiimide hydrochloride) (EDC), will tailor them as magnetic resonance (MR) imaging probes.

Toward Next-Generation Concentric Förster Resonance Energy Transfer Nanoprobes

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Förster resonance energy transfer (FRET) has been widely used as a sensing technique in biomedical research. Recently, quantum dot (QD)-based concentric FRET (cFRET) configurations have enabled multiplex sensing with a single nanoparticle vector. QDs are promising materials for bioanalysis owing to their excellent photoluminescence properties, small size, and versatile surface modification capabilities. To date, only cadmium-containing QD-based cFRET probes have been developed; however, cadmium often elicits fears of potential toxicity, which might limit the scope of such QDs. Therefore, this research aims to explore alternative materials for developing more biocompatible cFRET probes and expand the applications.

Polyamidoamine (PAMAM) dendrimer is a candidate material for developing cadmium-free cFRET nanoprobes. Non-fluorescent PAMAM dendrimers are useful as a core structure because their size is similar to that of a QD with multiple surface functional groups; however, a PAMAM dendrimer with luminescent materials. To this end, we labelled the dendrimer with luminescent terbium complexes to function as cFRET donor and replace the role of QD. Here, we report on the design, characterization, and proof-of-concept sensing applications for these novel dendrimer-based cFRET systems. Overall, our development of new and innovative cFRET architectures is a step toward a new generation of probes for biological applications.

Cellular uptake, cytotoxicity and trafficking of fluorescent carbon dots in human cells

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Carbon dots are nanoparticles with optical properties and have the potential for use in studies of cell physiology and medical applications. Although they tend not to be toxic, their fluorescence and cellular uptake are not well understood, and merit investigation. Here, we synthesized a fluorescent amine passivated carbon dots using microwave-assisted synthesis, and characterized it using UV-VIS spectroscopy, Fluorescence spectroscopy, TEM, FT-IR, XRD, and Zeta-potential to assess their physicochemical properties. We conducted further in vitro work in both HELA and HFF cells. We tested the effect of these carbon dots on cells viability, cellular uptake and sub cellular localization using live imaging epifluorescence microscopy. These studies suggest that these carbon dots are promising to pursuit and have great potential for use as imaging tools as well as drug delivery and carrier agents.

ABSTRACTS // ANALYTICAL CHEMISTRY SHOTGUN TALKS

Analyse des contaminants environnementaux dans les urines par LC-MRM

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Dans notre vie quotidienne, nous sommes exposés à de nombreux contaminants environnementaux qui n'ont pas de normes d'utilisation contrôlées mais qui pourraient avoir un impact sur la santé humaine et l'environnement, même à de très faibles concentrations. Les contaminants étudiés principalement de produits pharmaceutiques, d'additifs alimentaires, d'hormones, de produits de soins personnels, de plastifiants et de pesticides. Dans ce projet, nous développons une méthode bioanalytique pour quantifier ces contaminants environnementaux et leurs métabolites dans une matrice biologique telle que l'urine. Première, une méthode LC-MRM ciblée a été développée pour l'analyse de 34 contaminants de diverses structures chimiques. Ensuite, afin de quantifier ces molécules, une méthode d' extraction mini-QuEChERS est optimisée pour extraire efficacement ces molécules de l'urine. Cette méthode d'extraction, qui est Rapide, Facile, Pas Cher, Efficace, Robuste et Sûre, se fait en deux étapes : une extraction liquide-liquide par l'acétonitrile et les sels en premier lieu et une étape de nettoyage de la couche organique par extraction en phase solide dispersive (d-SPE) en second lieu. La méthode développée dans ce projet basé sur QuEChERS/LC-MRM permettra la détection et l'identification d'un large éventail de contaminants de polarité très différente dans des échantillons d'urine humaine provenant de volontaires. une extraction liquide-liquide par l'acétonitrile et les sels en premier lieu et une étape de nettoyage de la couche organique par extraction en phase solide dispersive (d-SPE) en second lieu. La méthode développée dans ce projet basé sur QuEChERS/LC-MRM permettra la détection et l'identification d'un large éventail de contaminants de polarité très différente dans des échantillons d'urine humaine provenant de volontaires. une extraction liquide-liquide par l'acétonitrile et les sels en premier lieu et une étape de nettoyage de la couche organique par extraction en phase solide dispersive (d-SPE) en second lieu. La méthode développée dans ce projet basé sur QuEChERS/LC-MRM permettra la détection et l'identification d'un large éventail de contaminants de polarité différente dans des échantillons d'urine humaine provenant de volontaires.

Untargeted metabolomic analysis of Hirschsprung's disease in a mouse model

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Hirschsprung's disease is a rare disorder affecting nerve cells in the intestine, causing obstruction of the colon, and has an incidence of 1/5000 births. There is a lack of neural ganglia cells in the lower colon. Certain children can present moderate symptoms such as constipation, while others can develop dangerous infections such as sepsis leading to major complications, including death.
Although, gene expression studies have shown that this rare disease involves several gene mutations, many factors are still unknown, hindering the development of therapeutic treatments. Further insight into the metabolic profile involved in this disease could provide insight into the development of the disease as well as provide potential biomarkers for therapeutic assessment.
We have conducted a preliminary untargeted metabolomic study of colon tissue from a mouse model of this disease and compared it to wild-type mice. Using liquid chromatography coupled to high resolution tandem mass spectrometry, we have found significant differences in metabolic features, some of which have been tentatively identified using spectral matching with metabolomic databases and accurate mass measurements. We will present results from this preliminary study and perspectives for future work in this presentation.

Modification of NaA Zeolitized Coal Fly Ash with Hexadecyl Trimethyl Ammonium Chloride as a Novel Adsorbent for Glyphosate Removal

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The purpose of this study is to develop a novel, efficient, and low-cost adsorbent for removal of Glyphosate (gly) from contaminated water. To accomplish this, NaA (LTA) zeolite was hydrothermally synthesized from Coal Fly Ash (CFA) as a waste material and then modified with Hexadecyl Trimethyl Ammonium Chloride (HDTMAC) cationic surfactant. Analytical instrumental methods such as ICP-OES, XRD, XRF, and FTIR were used to characterize zeolitized CFA and their modified forms. Preliminary results showed that the modified zeolite had a higher adsorption capacity than the unmodified zeolite at all pH values evaluated between 2 to 12. The glyphosate negatively and adsorbent surface positively charged thus the adsorbent performed well in acid pH ranges (2-3). The percentage removal efficiency was 97 percent in the acidic pH. Ion chromatography (IC) was used to measure the adsorption capacity of NaA-HDTMAC zeolite in the experimental design, and the results were 71 and 43 mg/g for pH 5 and 7, respectively. Different parameters such as contact time, initial concentration, and adsorbent doses, were optimized using Minitab software.

Fire history, vegetation and climate change in the Maya lowlands over 3,300 years

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Understanding past societal responses to climate change requires proxy indicators of human population, climate and land-use change. We apply a range of proxies to a lake sediment core from Laguna Itzan, a cenote adjacent to the ancient Maya population centre of Itzan, in order to examine the response of the lowland Maya to climatic and environmental change, which remains poorly understood. By combining molecular proxies for population (faecal stanols) and biomass burning (polycyclic aromatic hydrocarbons or PAHs) with isotopic analyses of plant wax n-alkanes as proxies for vegetation change ($\delta^{13}C$) and palaeohydrology ($\delta^{2}H$), we show the complex interplay of environmental and societal changes over 3300 years. Our data indicate that human population dynamics and patterns of land clearance for agriculture varied substantially throughout the sediment core record, and that palaeoclimatic change may have largely driven these patterns.

Ethanol fuel cell for clean environment

D. Alqdeimat
Memorial university

In general, greenhouse gases contribute to environmental problems like global warming. For this reason, it is necessary to improve and increase the use of renewable and clean energy sources with low net CO_2 production. The electrochemical oxidation of organic molecules such as; hydrogen, formic acid, methanol, and ethanol can be used as an alternative source of energy that decreases CO_2 emission. In recent years, direct ethanol fuel cells (DEFC) have been considered as an attractive power source with high potential for applications in vehicles and electronic devices. In spite of that, many problems have impeded DEFC implementation, including low current densities, incomplete ethanol oxidation, low faradic efficiencies, and crossover through the membrane. To overcome these problems, many anode catalysts have been developed to increase the activity, selectivity, and efficiency of DEFC. The main goal of my research focuses on the development of materials for energy conversion and storage. This will include preparing effective electro-catalysts for ethanol oxidation in direct ethanol fuel cells, in which turn increasing the efficiency and the performance of the cell. As a result, the DEFC will be commercially viable.

Review of current trends in Hydroxyapatite nano-particles for drug delivery applications – advantages and challenges

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Purpose: Hydroxyapatite (HA) is a material which possesses chemical composition similar to that of the mammalian hard tissues like bone and teeth. Therefore, it is widely used for various biomedical applications and extensive research has been carried out on HA based materials from decades. Nanotechnology helps to develop HA having dimensions in nanometer range. Nano-HA can be used as potential drug delivery carrier because of its excellent adsorption property, bio-similarity and non-toxicity. So, this review summarizes the recent advancement in the field of nano-HA based drug delivery systems. *In-vitro*, *In-vivo* and clinical trials were reviewed extensively on Nano-HA based drug delivery systems. Special consideration was given particularly to two major bone related fatal diseases namely bone cancer and bone tuberculosis(B-TB).

Methodology: PUBMED database along with the google scholar database were utilized for collecting and reviewing the existing literature. "Hydroxyapatite, drug delivery, drug carrier, Doxorubicin, Zoledronic acid, Methotrexate, Dactinomycin [FDA approved anticancer drugs], Streptomycin, Rifampicin, Capreomycin [Drugs for bone tuberculosis]" were used as keywords for finding and screening the existing literature. Specific attention was given to the recent literature published in last decade (2011-2021).

Polymer-Matrix Mediated Assembly of P3HT Nanowires

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Université de Montréal

Doped organic semiconductor polymer such as poly(3-hexylthiophene-2,5-diyl) (P3HT), shows a good electrical conductivity when it is in the form of nanowires and they are promising candidates in opto-electronic and energy conversion applications. However, conventional techniques, such as spin-coating, used to process materials containing polymer nanowires usually show low level of preferential orientations, and thus poor electrical properties for energy efficient applications. By using a non-traditional method, three-dimensional (3D) printing, and more specifically, direct-ink writing, we will explore if the alignment of P3HT nanowires can be enhanced via the shear forces experienced during the printing process. To facilitate the processing of the P3HT nanowires, the latter will be blended in a dielectric polymer matrix. We hypothesize that the phase separation between the polymer matrix and the nanowires, combined to the shearing forces experienced by the blend upon extrusion, will optimize the alignment of the nanowires with each other, thus leading to enhanced charge transport properties. The optical and thermal properties of the 3D printed materials, along with their morphology, will be characterized using UV-visible spectroscopy, differential scanning calorimetry and atomic force microscopy. Structure-processing-property-function relationships will be established to improve our ability to predict and control the 3D printing of pi-conjugated materials.

Powder X-Ray Diffraction Analysis of Cu/Cu_2O Nanocomposites Synthesized by Colloidal Solution Method

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The Cu/Cu_2O powder nanocomposites were successfully synthesized by colloidal solution method. To investigate the influence of oxidant agent concentration on the crystallite size and lattice constant of the nanocomposites, the X-ray diffraction method was utilized to collect the database for crystal growth analysis. Due to the imperfect crystal growth, the Nelson-Riley function and the Williamson-Hall method were used as to confirm the precise values of the nanocomposites. Using Rietveld refinement method based on the XRD pattern. The XRD results show that the diffraction peaks were mainly assigned to the cubic structure in good agreement with the JCPDS standards. Furthermore, the change

in oxidant agent concentration led to a very small change of microstrain in the peaks of Cu/Cu2O nanocomposites. Using these methods can aid in the precise study of the crystalline structure of the material, which can then be calculated to adjust the influencing conditions during the synthesis of the material.

ABSTRACTS // PHYSICAL CHEMISTRY SHOTGUN TALKS

Elucidation of proton dynamics and structure of an organic ionic plastic crystal employed in fuel cells using solid-state NMR

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Driven by the critical need to find alternatives to fossil-based fuels, fuel cell technologies offer relatively high efficiency, high-energy density and excellent scalability. Normally, an expensive Pt-based catalyst is used on the anode side. To lower the amount of Pt needed, our approach was to incorporate an organic ionic plastic crystal (OIPC) into a fuel cell catalyst. Cyclic voltammetry studies demonstrated that the OIPC-modified Pt/C catalyst had a significant improvement in oxidation of formic acid compared to the unmodified catalyst. Solid-state nuclear magnetic resonance (SSNMR) is a powerful tool that can provide information about the local structure and ion mobility. Different SSNMR experiments were performed including one-dimensional variable-temperature ^{1}H MAS NMR, ^{1}H-^{31}P MAS cross polarization NMR, ^{1}H-^{31}P heteronuclear correlation (HETCOR). ^{1}H-^{31}P HETCOR provides information to accurately assign the 1D spectrum and determine the local structure of the cation.

The Exploitation of Molecular Perturbation Effects in Experimental and Calculated Vibrational Spectroscopy

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Previous research determined that adding perturbing molecules to a thin film affected the infrared spectrum in a similar manner to matrix isolation experiments: compared to an unperturbed spectrum, the perturbed spectrum was shifted and the intensity for certain peaks was decreased. Upon further analysis, these effects were found to be isolated to –CH_3 groups at the tail of the self-assembled monolayers. An algorithm was previously designed to subtract this “surface” spectrum from the bulk spectrum of thin films, however, it relied on user defined parameters.

Alkanethiol self-assembled monolayers containing both an odd and even number of carbons of varying chain lengths have been explored with perturbing molecules varying in polarizability. Trends in odd films show the backbone of alkanethiol films are affected when perturbing molecules are added, albeit to a lesser extent than the surface group. Short-chain films follow similar trends to their long-chain counterparts. Increasing the polarizability of perturbing molecules increases the shift and scale in the spectrum. Through continued analysis of films before and after perturbation, experimentally and computationally, this project aims to refine the algorithm to isolate the surface spectrum of any given thin film using infrared spectroscopy.

Phase behavior of 2D self-assembled phospole-lipid films

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Π-conjugated systems containing heteroatoms have shown interesting properties and are used in production of practical materials such as organic sesnsers. Lipid compounds with phosphorus-based π-conjugated head groups with both electronic and amphiphilic character have shown strong intermolecular interactions, leading to well-oriented liquid crystal structures. The major contributor to the highly directional, self-organization driven by non-covalent interactions is thought to be extensive π-stacking among the aromatic rings.

In this work, the 2-D self-assembly in Langmuir and Langmuir-Blodgett monolayers of a series of phosphole-lipids at the air-liquid and air-solid interfaces is explored. Their structural organization and phase behavior is evaluated using surface tensiometry, Brewster angle microscopy, imaging ellipsometry, atomic force microscopy, and grazing incidence x-ray diffraction. The properties and stability of different phases along the isotherm will be evaluated to probe the role of intermolecular π-stacking.

ABSTRACTS // INORGANIC CHEMISTRY SHOTGUN TALKS

Cavity-Containing Anionic Salicylic Acid-Based Metallostructures: Interplay Between Methylene and Aromatic Bridges in Ditopic Ligands

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The versatility and relevance of metallostructures in the field of supramolecular chemistry have contributed significantly towards our understanding of self-assembly, molecular recognition, interactions with biologically relevant molecules, catalysis, and design of therapeutics. Studies on these materials, however, have largely focused on cationic and neutral systems. Studies on the preparation of new anionic structures as functional materials and for guest binding are scarce.

Herein, we disclose the design of a new class of anionic metallostructures assembled from tri- and tetravalent metal cations in the presence of ligands derived from salicylic acids. We demonstrate the nuances of their self-assembly in the presence of various inorganic and organic cations, as well as the importance of the interplay between methylene and aromatic bridges in order to obtain structures with accessible cavities for potential host-guest interactions. We further discuss the implications on the discovery of new solid and functional materials.

Conversion of electrochemically deposited carbonates to perovskite with retention of crystal morphology

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

Arrested Development: Stabilization of an Aromatic Primary Hydroxylamine Function Upon Coordination with Transition Metal Ions

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Aromatic compounds containing a redox-active hydroxylamine functionality (Ar-NH-OH) are of great interest due to their intrinsic reactivity, redox properties, involvement in biological processes, and their potential to act as catalysts. For example, arylhydroxylamines can act as a nitric oxide donor in mammals under certain conditions. Despite their great potential for redox conversions, the high reactivity of these compounds has left this area of study severely underdeveloped, with only a few examples of metal complexes with chelating *alkyl*hydroxylamines presented in literature. Herein, we present a series of crystallographically characterized complexes with redox-active metals and an intact aromatic primary hydroxylamine function that are among the first of their kind.

Here we show that proper ligand design allows for the stabilization of these complexes contrary to the common belief that arylhydroxylamines decompose or disproportionate in the presence of transition metal ions. Through meticulous ligand design, we produced two different ligands containing hydroxylamine functions that allowed for high yield preparation of zinc, nickel, and copper complexes that are stabilized via intramolecular hydrogen bonding. The metastability of these complexes allows for a careful, methodical study of their electronic properties, reactivity and implication as catalysts in organic oxidation reactions.

Copper-MOF Electrocatalyst System for an Integrated CO_2 Capture and Conversion

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Carbon dioxide concentration in the atmosphere is caused by the fossil fuels and natural gas combustion used in power generation, transportation and industrial processes. Here, we developed an integrated device, where our in-house MOF, which adsorbs CO_2 in presence of water, serve as CO_2 concentrator and copper-based nanostructured catalyst electrochemically converts CO_2 into valuable C_2^+ based products. The MOF and Cu catalyst, which are supported in a carbon fiber sheet that acts as a platform to conduct the current, facilitates the CO_2 capture and the electrochemical reduction reaction of CO_2, respectively. One side of the carbon fiber is coated with the zinc-based MOF with 500 m^2/g Langmuir surface area, and an adsorption capacity of 4 mmol/g CO_2 at 20°C. The MOF layer served as a CO_2 concentrator, allowing a higher percentage of CO_2 molecules to pass through the fiber to the other side, where the CuO particles catalyze the electrochemical reduction reaction. Binary gas feed 50%/50% N_2/CO_2 was used for the electrochemical reduction experiments in a flow-cell configuration. The results showed high C_2^+ products selectivity such as ethylene, conversion efficiency, and catalyst stability.

Electrocatalytic Generation of H_2 from Water with Zn(II) Complexes Displaying Cooperative Ligand Reduction

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Hydrogen is a promising and environmentally benign energy carrier. One of the promising techniques for H_2 production is electrolysis. Among the 3d metals, perhaps not surprisingly, Zn is nearly absent from the metals that have been used for catalytic hydrogen production. The key obstacle to using Zn is that is found almost exclusively in the 2+ oxidation state and this redox innocence blocks ability to undergo the fundamental of oxidative addition and reductive elimination steps typical of homogeneous catalyzed reactions.To our knowledge, there are only two reports for hydrogen generation using molecular Zn catalysts. These species in which these catalysts displayed catalytic reduction currents at −2.3 V and −3.29 V *vs* $Fc^{+/0}$ in the presence of acetic acid as proton source through ligand-centered pathways. Water represents the most sustainable source for H_2 production and the efficient electrocatalytic production of H_2 from mixed water/acetonitrile solutions by using two air-stable Zn(II) pincer complexes, $[Zn(k^2\text{-}\{Ph_2PNMe\}_n(NC_5H_3)Br_2]$ (n=1 I, 2 II) is reported. Hydrogen generation from H_2O/CH_3CN solutions is initiated at -2.3 V *vs* $Fc^{+/0}$, and bulk electrocatalysis studies showed that the catalyst functions with an excellent Faradaic efficiency.

Cobalt based transition metal spinel oxide thin films as efficient water oxidation electrocatalysts

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Hydrogen is viewed as one of the energy carrier of the future as it is environmentally friendly, inexhaustible and possesses high energy density. Water electrolysis is an efficient and sustainable way to produce hydrogen. However, the practical application of water electrolysis is limited due to its high cost, which is related to the high overpotential associated with oxygen evolution reaction (OER) at the anode. Cobalt based spinel metal oxides are potential candidates for OER due to their excellent catalytic properties and stability in alkaline medium. We have prepared various spinel oxides, namely $Cu_xCo_{3-x}O_4$ (x = 0 to 1), $Ni_{1-x}Cu_xCo_2O_4$ (x = 0 to 0.75), $Fe_yCu_{x-y}Co_{3-x}O_4$ and $Fe_yNi_{x-y}Co_{3-x}O_4$ (y = 0.1 or 0.15 and x = 1 or 0.5) using the thermal decomposition method. The films were analyzed, using several structural, chemical and electrochemical methods such as X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX), cyclic voltammetry and X-ray photoelectron spectroscopy (XPS). Electrochemical measurements show that the electrodes exhibit overall good catalytic activity towards OER. However, addition of small amount of Fe to form $Fe_yCu_{x-y}Co_{3-x}O_4$ and $Fe_yNi_{x-y}Co_{3-x}O_4$ show a significant enhancement, indicating these compositions could be good candidates for OER.

Exploring the Chemistry of Phosphorus Hydrazonides

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The development of electronic devices and technologies, such as solar cells and fluorescent dyes for used chemical biology, rely upon the continued discovery of molecular optoelectronic materials. Archetypal examples of molecular materials utilized in these applications often contain a boron difluoride unit chelated by a π-conjugated *N*-donor ligand. The coordination of heavier main group elements in place of boron has led to unique optoelectronic and redox characteristics when chelated to a conjugated *N*-donor ligand and can thus be used as an additional tool to tailor the resulting properties. Despite limited presence in the literature, the incorporation of phosphorus has resulted in desirable properties such as water solubility, and a facile synthesis to low reduction potentials and donor-acceptor characteristics. Phosphorus hydrazonides have been scarcely reported, but their optoelectronic properties remain underexplored. The feasibility of phosphorus hydrazonides as an emerging class of molecular materials will be assessed, and recent results concerning their synthesis, characterization and optoelectronic properties will be shared.

ABSTRACTS // ORGANIC CHEMISTRY SHOTGUN TALKS

Synthesis of analogues of PS–3114, a non-nucleoside inhibitor of DNMT3A

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DNA methylation is a stable epigenetic modification that leads to the installation of a methyl group at position 5 of cytosine. Deregulation of DNA methylation processes has been observed in several types of cancer leading to inhibition of promoter regions of tumor suppressor genes. It has been found that this change can be reversed by inhibiting DNMTs. Currently, the only approved drugs that target DNMTs are Vidaza and Dacogen for the treatment of myelodysplastic syndrome. However, these drugs which have a nucleoside-like structure have poor bioavailability, are non-selective and are cytotoxic since they rely on a mechanism involving incorporation into the genome. Thus, there is an urgent need to develop new potent non-nucleoside inhibitors of DNMTs that have good biophysical properties and minimal toxicity. Our group recently identified by an NMR fragment screening PS-3114, a small molecule with an IC_{50} of 65 µM against DNMT3A. In this presentation, we will show our advancement on the synthesis of derivatives of PS–3114 and the evaluation of their potency by fluorescence and 3H-SAM radioactivity tests.

Synthesis of Multi-Substituted Furans from Renewable Platform Chemicals

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With climate and environmental concerns consistently growing, the chemical industry is bound to shift away from petroleum resources and turn to sustainable feedstock derived from biomass. There is urgency to develop new methods to convert biomass into consumer-useful products efficiently. Hydroxymethylfurfural (HMF) is a biomass-derived platform chemical that has received much attention due to its renewable obtainability and chemical functionality to produce various bulk chemicals. This project aims at creating a versatile methodology to transform HMF into multi-substituted furans through palladium catalysis. Versatility of this methodology comes from the ability to regioselectivity install a variety of aryl groups at specific locations of the furan base. Methods of chemical installation are driven by two excellent reactions that facilitate new sp2–sp2 carbon bond formation between two aryl molecules: palladium-catalyzed decarboxylative cross-coupling and Suzuki-Miyaura cross-coupling reactions. Production of multi-substituted furans can be seen in their applications for organic semiconductors and OLEDs, due to the optoelectronic properties found in highly conjugated furans.

Exploring Ellagic Acid as an Organic Semiconductor

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Organic semiconducting (OSC) materials have been studied extensively in the field of electronics as they provide a gateway to fabricate devices that are smaller, more flexible, and easier to process in comparison to their inorganic counterparts. In the past decades, researchers have been investigating new OSC materials that can act as efficient semiconductors all the while being produced in a sustainable manner without extensive synthetic methodologies. Ellagic acid (EA), a natural polyphenol found in a variety of plants, represents an ideal candidate to become a sustainable organic semiconducting building block. Its natural abundance and its underexplored performance as an organic semiconductor leave great room for future advancement in using this molecule as a core building block for organic electronic purposes.This shotgun presentation will focus on the functionalization of EA's peripheral hydroxyl groups with aryl moieties through S_NAr reactions, providing a facile two-step approach to tailor the electronic properties of the material by expanding its π-conjugation. Although this work is still ongoing, initial results obtained from the pyrazine and quinoxaline derivatives have shown promising data for the fine-tuning of EA's electrochemical properties to act as a OSC active material.

Synthesis of fluorescent analogues as mutated 1DH1 sensors for guided surgery of gliomas

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Gliomas are graded primary brain tumours, where higher grades are associated with more aggressive treatment and reduced 10-year survival rates. Typical treatment options include surgery, chemotherapy, or radiotherapy. More than 80% of adult grade II and III gliomas contain isocitrate dehydrogenase (IDH1) mutations, most frequently the exchange of wild type (WT) Arg^{132} to His^{132}. The role of WT-1DH1 is to catalyze the oxidative decarboxylation of isocitrate to alpha-ketoglutarate (αKG) whereas the mutated reaction irreversibly converts αKG to D-2-hydroxyglutarate (D-2HG), leading to accumulation of 5 to 35 µmol/g of tumour. The mutation of IDH1 occurs early in the development of brain tumours, thus presenting an opportunity to detect tumours earlier for intervention. Hence, we propose to design a D-2HG analogue as a real-time diagnostic marker.

Our approach is the design of a responsive fluorogenic analogue of aKG, which when processed by IDH1, will release a modified fluorophore with a distinct bathochromic shift. Analogues were designed and screened *in silico* including docking simulations, then developed synthetically.

A potential application of this work would be fluorescence-guided surgery wherein malignant tumours are distinguished *via* the high concentration of D-2HG. This will lead to improved survival rates and greater treatment options for glioma patients.

Diversifying the pseudoproline library to facilitate access to microcyclic peptides

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Peptides are bioactive oligomers of amino acids and along with their larger congeners, proteins, are involved in virtually every biological anabolic and catabolic process. As drug discovery is shifting towards inhibiting protein-protein interactions, peptides, and especially cyclic peptides, are many of the best congeners.

Peptide cyclization is an important posttranslational modification that confers several advantages: peptidase-catalysed digestion is significantly slowed; bioavailability and cell penetration are improved.

One particularly powerful method relies upon the conformational bias imparted by prolinyl residues,which pre-arranges the peptide chain for cyclisation; however, this is limited by the need for a multiple prolines as part of the amino acid sequence.

The Trant Team is looking to address this challenge by incorporating a removable group into the amino acid side chain that enables the formation of novel pseudoprolines. Initially we seek to target the four aromatic amino acids.Making use of the reactivity imparted by the aromatic ring, these amino acids will be selectively functionalised with a β-hydroxyl group by a bromination/substitution sequence. This β-hydroxyl group can then be used to form the pseudoproline with the α-amino group, which will then be Fmoc protected and utilised in solid-phase peptide synthesis. This presentation discusses our initial work towards these targets.

Metal Coordination of a Self-Assembling Histidine-Based Fatty Acid-Peptide Conjugate

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Life and its complex biological systems stem from self-assembly of individual molecules into higher order structures. Non-covalent interactions, such as π-π stacking, hydrogen bonding, and hydrophobic interactions, drive the spontaneous molecular recognition allowing for the formation of supramolecular structures. This recognition is fundamental to cellular function, such as protein-folding and enzymatic activity, as well as structural integrity, such as membranes and cytoskeletons. Peptides, as these protein precursors, are highly studied for molecular recognition and supramolecular assembly. Histidine is a highly prevalent amino acid examined in the functional components of such structures, as it is often a catalytic residue in enzyme active sites. It is also well known to coordinate to metal ions, thus presenting an interesting opportunity to investigate histidines role in the context of structural integrity in self-assembled molecular structures. We examine a simple histidine-based fatty acid-pepide conjugate and characterize the structural morphology and mechanical properties of its self-assembled supramolecular hydrogel. We introduce divalent metal ions for coordination as a potential method to modulating the assembly mechanism, which would therefore alter the resulting nanostructures and its mechanical properties.

Icephobic Coatings for Aerospace Applications

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Icing and ice accretion on aerodynamic surfaces can have severe detrimental impacts on aircraft and impose limited operability particularly to small and light aircraft. Passive ice protection coatings are being actively pursued to reduce the potential safety hazards and property damage caused by icing; however, they still fail to achieve the simultaneously high icephobicity and durability required for aerospace applications.

Novel gel-like fluoropolymers were prepared and incoporated into hydrophobic polyurethane (PU) elastomers to produce coatings and thin films with a high fluorine content on the surface. The mechanical properties and high icephobicity of these coatings was determined through experimental testing. These coatings exhibited high water contact angles, good tensile strength, and impressive durability against sand erosion; however, small water droplets did not slide easily on the surface suggesting the water-coating interactions present may limit the level of icephobicity achievable with this material.

The results of the experimental study found PU to be the ideal material for developing future icephobic coatings for aircraft applications. These findings also direct the next wave of icephobic coating development towards the formulation of new, innovative solutions capable of reducing PU-water interactions and suppressing ice formation on the coating surface to achieve the desired high icephobicity.

Development of New Small-Molecules TEAD Inhibitors Derived from Flufenamic Acid

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

Liesegang patterns of copper aspartate coordination polymer in gels

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Self-assembly of metal ions and amino acids to form coordination polymers is well known. In the past, coordination polymers have been mostly synthesized via solvothermal methods. Herein, the crystallization of coordination polymers in gels is investigated. Crystal growth in gels is dominated by diffusion and often leads to high quality single crystals. We demonstrate the green synthesis of copper aspartate in agar gel which leads to coordination polymers with spherulitic morphology. Remarkably, crystallization of copper aspartate in gel also displayed Liesegang banding. This phenomenon results in a series of repeating concentric bands. The Liesegang ring phenomena was optimized by investigating various parameters, including amino acid and Cu2+ concentration, chirality, and solvent. The coordination polymers were characterized by scanning electron microscopy, circular dichroism, powder X-ray diffraction, infrared spectroscopy and light microscopy. A size gradient of spherulites was observed, where the spherulites are smaller at the interface but increase in size going down the testube which is characteristic of crystallization in gels. Interestingly, SEM images showed that the overall width of the nanofibers incorporated within the spherulites decreased going away from the interface. Depending on the chirality and the difference in the solubility of the homochiral and the racemic aspartic acid, the banding pattern was quiet different. In the case of the homochiral aspartic acid, the coordination polymer formed more bands that were thinner in size. Whereas, the racemic copper aspartate formed fewer bands but they were thicker. Furthermore, results from solid state CD and PXRD indicate no conglomerate coordination polymer formation starting from racemic aspartic acid. The crystallization of racemic 1-phenylethylamine with transcinnamic acid, known to form chiral conglomerates, is currently being investigated in gels as a possible means for spatial spontaneous resolution.

Identification, subcellular localization and topology of AltSLC35A4, a highly abundant alternative protein in vertebrates

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BACKGROUND: Alternative Open Reading Frames (altORFs) provide a new source of protein diversity in eukaryotes, allowing expression of multiple proteins from a single mature mRNA. The expression of thousands of altORFs-encoded proteins alternative proteins) has been experimentally validated, and several of them have important biological functions. However, most alternative proteins are still largely uncharacterized and unknown. This is the case of the one produced by the double-coding gene *SLC35A4*, which encodes in its 5'UTR one of the most abundant and conserved alternative proteins in vertebrates, AltSLC35A4. OBJECTIVE: To determine the subcellular localization and topology of AltSLC35A4. METHODS & RESULTS: In order to determine the localization of AltSLC35A4 with immunofluorescence, a test of colocalization with organelle markers has been used on cultured human cells (HEK293T, 143B). Our preliminary data suggest that AltSLC35A4 is located in peroxisomes. Then, a transmembrane domain in AltSLC35A4 was predicted using TMHMM software. Its membrane insertion was validated by alkali treatment followed by Western blotting. Finally, the topology of AltSLC35A4 was determined using immunofluorescence following differential permeabilization of plasma and peroxisome membranes with digitonin. CONCLUSIONS & PERSPECTIVES: We aim to generate knockout cells for AltSLC35A4 in order to identify the functional and cellular role of our protein.

A new approach to plastic recycling: the use of enzymes in moist-solid reaction mixtures

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McGill University

Plastic is essential to our daily lives, and as a result, we produce millions of tons of plastic every year. Unfortunately, only a very small fraction of plastic is recycled, and the recycling processes available are not efficient. The use of enzymes as natural catalysts for plastic degradation presents an exciting opportunity for an environment-friendly recycling that can break plastics down to their monomers, while avoiding the use of harsh chemicals or conditions. Recently, our group developed a novel technology that uses enzymes in mechanically mixed moist-solid reaction conditions. While dramatically different from the dilute aqueous reaction mixtures in which enzymatic reactions typically take place, this technology has proven very efficient for the depolymerization of highly crystalline polyethylene terephthalate as well as other polymers such as cellulose and chitin. Depolymerization proceeds without any harsh chemical or thermal pre-treatment of the material and with only few equivalents of water, minimizing the amount of solvent waste. With the goal of expanding upon this technology and applying it more widely to other plastics, my project represents an important step towards achieving a circular plastics economy and therefore an important step towards tackling plastic pollution.

The Role of HuR in Adult T-Cell Leukemia/Lymphoma

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Adult-T-cell Leukemia/Lymphoma (ATLL) is a rare disease caused by infection with the human-T-lymphotropic type-I (HTLV-I) retrovirus. In Canada, Quebec has the largest number of reported ATLL cases. Current cancer therapies have been ineffective at treating this disease. There is therefore an urgent need to uncover the molecular mechanisms that drive ATLL, to provide insight for the development of novel therapies. Transformed T-lymphocytes are characterized by the dysregulation of the immune response and apoptosis to promote tumor progression. Upregulation of Programmed cell Death 1 Ligand (PDL1) is one way in which tumor cells escape immune surveillance. Recent studies have shown that upregulated expression of PDL1 can be mediated post-transcriptionally by the RNA-binding protein, HuR. Interestingly, HuR has also been shown to regulate the apoptotic response through its caspase-mediated cleavage. The caspase-

mediated cleavage of HuR occurs at residue D226, the mutation of which prevents apoptosis. Recently, a mutation in HuR (HuR-V225I) was identified in patients with ATLL near HuR's apoptotic cleavage site. This study aims to identify the causative role of HuR in ATLL by assessing its role on the post-transcriptional regulation of PDL1, as well as its involvement in apoptotic resistance, and the effect the mutation, HuR-V225I, has on these roles.

Dynamics of the evolution of antibiotic resistance in soft agar

L. Domínguez
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Antibiotics have revolutionized medicine since their discovery in the 1920's; saving countless lives. Unfortunately, over 2 million people are infected with antibiotic-resistant bacteria each year, causing more than 23,000 deaths in the US alone. According to current predictions, by 2050, antibiotic-resistant bacteria will cause 10 million deaths worldwide each year. While resistance conferred by mutations can be easily monitored under laboratory conditions, little is known about the dynamics of this evolution, especially at the single cell level. Using a soft agar gradient evolution system, we will characterize how *de novo* mutations arise in bacterial populations and in single cells. Antibiotic resistance is an inherent consequence of antibiotic therapy. However, by understanding how these resistance mutations arise, as well as the conditions that result in dead-end lineages, we will be able to predict resistance before it arises in the clinic and adjust our therapeutic approach to compensate. Better therapeutic options could then help save tens of millions of lives and trillions of dollars each year, prolonging the effective use of antibiotics far into the future.

Discovery of atypical SUMO E3 Ligases in humans through biochemical and bioinformatics approaches

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UQAM

Post-translational modifications allow cells to adapt to their environment by altering protein characteristics such as localisation, stability, inter-proteins interactions. SUMOylation is a reversible post-translational modification involving a covalent bond between a protein named SUMO and a protein substrate. This modification occurring mainly in the nucleus, involves the action of three proteins: E1 to activate SUMO, E2 to conjugate SUMO and E3 to transfer SUMO on a specific substrate. SUMO E3 ligases are differentiated by the presence (typical ligases) or absence (atypical ligases) of a RING domain that facilitates interaction with a SUMO-loaded E2. ZNF451 is an atypical ligase containing 2 SUMO interacting motifs (SIM) that are sufficient and necessary to facilitate the transfer of SUMO on substrates. Our hypothesis is that there are other atypical SUMO E3 ligases that use small structural elements like SIMs to SUMOylate proteins. Our objective is to identify, purify and characterize other proteins which could possess SUMO E3 ligase activity. Our bioinformatics studies so far suggest that ZNF24 could possess such activity. We were able to express and purify this protein and are currently characterizing it. Overall, this study will provide a better understanding of the molecular mechanisms that allow cells to regulate protein activity.

Structural and molecular characterization of the interaction between SIZ1, a SUMO-E3 ligase involved in Arabidopsis thaliana environmental stress responses, and its substrates

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Protein post-translational modifiers such as Small Ubiquitin-like Modifier (SUMO) play a key role in plant response to environmental stresses such as high temperatures, drought, and flood. Proteins are SUMOylated through an enzymatic cascade involving an E1 activating enzyme, an E2 conjugating enzyme and E3 ligases that bring substrate and SUMO-charged E2 in a complex that facilitates transfer of SUMO to a target lysine residue. Although several hundreds of substrates have been identified in model plants such as *Arabidopsis thaliana* - notably in response to environmental stresses - the precise molecular mechanisms of substrate selection remain elusive. Our hypothesis is that both protein-protein and protein-DNA contacts contribute to substrate recognition by SUMO E3 ligases. Our objective will be to elucidate the molecular determinants of E3-Subtrate and DNA-E3-Substrate interaction in *Arabidopsis thaliana*. To do so, recombinant E1, E2, E3, SUMO and substrates were obtained using heterologous protein expression in *E. coli*. The importance of specific protein and DNA interactions will soon be assessed using *in vitro* SUMOylation essays. Given the implication of SUMOylation in plant response to environmental stress, a better understanding of E3-Substrate interactions would pave the way to the production of more resilient crops through molecular engineering or selection.

Optimizing Small-Molecule inhibition of Systemic Juvenile Idiopathic Arthritis (sJIA) and Macrophage Activation Syndrome (MAS) Biomarker Interleukin-18 (IL-18) via Autodock Vina and Swiss ADME

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Systemic juvenile idiopathic arthritis (sJIA) is a subtype of JIA characterized by systemic joint inflammation and chronic fever upon onset. It affects 10-20% of children with JIA. While sJIA has no known cause, there are known biomarkers, notably high concentrations of proinflammatory cytokines interleukin-1, interleukin-6, and interleukin-18 (IL-18). Currently, there are anti-interleukin-1 and anti-interleukin-6 treatments but no anti-IL-18 treatments approved for sJIA. In sJIA, IL-18's free concentration is elevated, especially in patients with a history of macrophage activation syndrome (MAS). As a result, IL-18 neutralization serves as a potential treatment for sJIA patients non-responsive to previous treatment or those who have experienced MAS. Prior to research under the Oklahoma Center for the Advancement of Science and Technology, there were no published small molecules inhibiting IL-18's bioactivity. They proposed compounds NSC201631, NSC80734, and NSC61610 as potential inhibitors of IL-18 Binding Protein and IL-18Rα binding to IL-18. In this project, these small-molecules were docked using Autodock Vina. Novel analogs of them were designed and docked. The drug viability (i.e. solubility, lipophilicity, bioavailability) of each small-molecule was predicted using Swiss ADME. The results of the binding and viability tests were compared and will aid in developing drug therapies for sJIA and MAS patients.

Amyloid peptide to guide the self-assembly of perylene diimide into functional nanostructures

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Perylenediimides (PDIs) are one of the most relevant organic dyes that have been largely exploited owing to their excellent chemical robustness, stability, and optoelectronic properties. Therefore, PDIs have been extensively applied and used in various biomedical and nanotechnological fields. However, the precise control of their molecular self-assembly into a highly ordered supramolecular nanomaterials remains problematic. In this study, we took advantage of the high aggregation propensity of amyloid peptides to design nanofilaments functionalized with PDI. The amyloidogenic domain of the islet polypeptide, i.e., the segment 20-29 ($S_{20\text{-}29}$), was used as the self-assembling motif, which was connected to PDI by a flexible hexyl spacer. A symmetric (PDI-$[S_{20\text{-}29}]_2$) and asymmetric (PDI-$S_{20\text{-}29}$) hybrid peptides were prepared, and their self-assembly process in aqueous buffer was periodically followed by measuring absorbance and fluorescence of PDI, by circular dichroism spectroscopy and by atomic force microscopy. The analyses revealed that both PDI-peptides self-assembled into long, unbranched, and linear filaments with a cross-β-sheet quaternary organization. The UV-vis absorbance spectra exhibit a clear signature of H-aggregates for both assemblies. Overall, this study exposes that defined

nanostructures functionalized with PDI can be obtained from amyloid peptide building blocks, opening to novel applications in bioimaging, photodynamic therapy and bioelectronic.

Systematic review of collagen biochemical properties in osteogenesis imperfecta

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Osteogenesis imperfecta (OI) is a rare connective tissue disorder characterized by bone brittleness and caused by a mutation in type 1 collagen encoding genes or collagen processing genes. The severity of OI can vary drastically between the 18 different genes involved in pathogenesis. Studies relating OI genotype to phenotype severity were unable to find a correlation between them. We hypothesis that the biochemical properties of the type 1 collagen are dependant of the severity of OI. The objective of this systematic review was to systematically identify all studies measuring the biochemical properties of type I collagen in OI. In addition, patient information such OI type, age and sex will be used as covariates. Academic paper which measured quantitatively lysine hydroxylation, proline hydroxylation, hydroxylysine glycosylation, melting temperature of collagen and collagen secretion were selected. The academic database Medline and Embase were used and 701 unique papers were identified. Thus, the data includes diverse patient population with regards to OI type. Gaps in knowledge in regard to patient age and sex reporting is identified. Nevertheless, our study demonstrates that meta-analysis for several outcomes related to collagen biochemical properties is feasible.

Molecular tools to enhance protein SUMOylation: development and application in Rett Syndrome

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SUMOylation is a post-translational modification allowing the conjugation of a protein, Small Ubiquitin-Like Modifier (SUMO), on a target protein. This modification is involved in a variety of biological functions such as DNA repair and transcription regulation. Many evidence points towards SUMO's involvement in the biological activity of the Methyl CpG Binding Protein 2 (MeCP2), a transcriptional regulator associated with the repression of target genes. Various mutations on MeCP2 are known to cause Rett syndrome, a neurological disorder occurring in 1/10000 women and leading to severe cognitive and motor impairments. These mutants all share a decrease in SUMOylation caused by a loss of affinity between MeCP2 and PIAS1, a SUMO E3 ligase. In turn, this could contribute to a loss of MeCP2 activity and contribute to the severity of Rett syndrome. Our hypothesis is that re-establishing MeCP2's SUMOylation could alleviate some of the symptoms of Rett syndrome. This project thus aims to develop molecular tools allowing the SUMOylation of target proteins such as MeCP2 to better understand the role of SUMOylation on MeCP2's function and provide new therapeutical strategies for diseases such as Rett Syndrome.

Drosophila Microtubule Dynamics Show High Rescue Rate and Low Nucleation Threshold

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Microtubules are dynamic protein polymers found in all eukaryotes. They have largely been studied in mammals, but recent progress in tubulin purification has finally made it possible to purify it from any eukaryotic source. Microtubules characteristically display dynamic instability: stochastic switching between growth and shrinkage. Dynamic instability is described by 4 measurements: the growth rate, the rate of switching to shrinkage (known as "catastrophe"), the shrinkage rate, and the rate of switching back to growth (known as "rescue"). Tubulin, the building block of microtubules, has high overall conservation (89-95% for α-tubulin, 88-94% for β-tubulin), making it easy to pin down how specific sequence changes in the tubulin dimer are correlated with changes in the polymer dynamics. I characterized the dynamics of microtubules from Drosophila melanogaster and noted unique dynamic differences. I observed that Drosophila microtubules begin to grow at lower tubulin concentrations than mammalian microtubules (1.5 uM and 5 uM, respectively). Additionally, while reconstituted mammalian microtubules rarely rescue, these events are present with high frequency in Drosophila microtubules. Comparing my new dataset to existing results from mammals like Bos taurus, the worm Caenorhabditis elegans, and the yeast Saccharomyces cerevisiae will help us understand how microtubule dynamics differ across species.

One step purification and regulation of fructose 1,6-bisphosphatase in the liver of freeze tolerant wood frog, Rana sylvatica

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The wood frog (*Rana sylvatica*) undergoes numerous changes to its physiological and metabolic processes to survive in winter months. The wood frog drops its metabolic rate drastically to limit the use of energy during freezing conditions. The regulation of key enzymes plays a critical role in alterations of central metabolic pathways. Fructose-1,6-bisphosphatase (FBPase), was characterized in the present study during freezing in liver. It is a crucial enzyme of gluconeogenesis. Purification of FBPase to homogeneity from wood frog liver was performed in control and frozen wood frogs by a one-step chromatographic process. FBPase was subsequently assayed to determine the kinetic parameters of the enzyme. Studies revealed the relative degree of posttranslational modifications in FBPase from control and frozen frogs. Further, this study demonstrated a significant decreased sensitivity to its substrate fructose-1,6-bisphosphate (FBP) in frozen form when compared to the control. Immunoblotting demonstrated decreasein serine phosphorylation (53%) in the frozen FBPase. Taken together, these results suggest that FBPase is suppressed, and gluconeogenesis is inhibited in freezing. Therefore, this response acts as an important metabolic survival strategy of the wood frog.

Acetylation of Hemoglobin and its Effects on Protein Function and Structure

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Hemoglobin, the protein primarily responsible for oxygen transport, exists in two states: the high oxygen affinity R (relaxed) state, and the low oxygen affinity T (tense) state. Under normal physiological conditions, the equilibrium lies strongly in favor of the more stable R state. Consequently the T state requires the presence of allosteric modulators – namely, 2,3-diphosphoglycerate (2,3-DPG) – for stabilization.1 Here, we present a possible means of stabilizing the T state of hemoglobin through chemical modifications only (thus in the absence of allosteric modulators), specifically by use of the simple acetylating agent methyl acetyl phosphate (MAP).2 Mutiple experimental results demonstrated that acetylating the protein produced properties that perfectly resemble the T state of hemoglobin: namely reduced oxygen affinity and reduced cooperativity. We observed that hemoglobin acetylation was inversely proportional to oxygen affinity, suggesting a conformational shift towards the T state. Furthermore, we observed a decrease in cooperativity associated with increased acetylations similar to that observed when 2,3-DPG binds to hemoglobin. More importantly, although we saw decreased cooperativity (n50 = 1.8 versus 2.8), the protein remained cooperative (n50 > 1) – a property of hemoglobin essential for effective oxygen transport. Even upon peracetylation of the protein, it remained cooperative and able to bind oxygen. Therefore extensive acetylations did not destroy the proteins function. To confirm that these T state-like properties are indeed caused by a conformational change, we plan to conduct CD and UV-Vis spectroscopic studies for conclusive evidence. We are also interested in determining if these altered properties are site-specific (acetylation of certain specific sites cause more profound effects) through future peptide mapping experiments.

Effects of lanthanide-doped upconverting nanoparticles on nuclear biomarkers

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Upconverting nanoparticles (UCNPs) can generate high energy photons through the absorption of multiple photons of lower energy through a process known as photon upconversion. Lanthanide-doped UCNPs (Ln-UCNPs) are a class of nanoparticles that have unique physio-chemical properties. These features are ideal for biological and medical applications. Accordingly, Ln-UCNPs have emerged as promising tools for theranostics. However, the bio-nano interactions of Ln-UCNPs are poorly understood. This knowledge gap has limited the use of Ln-UCNPs in living cells.

Nuclear homeostasis is essential to cope with stress, such as the exposure to nanomaterials. Our research defines the impact of Ln-UCNPs on cell physiology, as it relates to nuclear biology and stress responses. To this end, we are assessing the effects of Ln-UCNPs on cell viability, the localization and abundance of key components of the nucleus, and the damage to this organelle. Our work provides a quantitative readout for stress responses, proteostasis, and cell organization in Ln-UCNP treated cells. Non-malignant fibroblasts and cancer cells serve as main model systems.

Collectively, our experiments determine the biocompatibility and subcellular interactions of Ln-UCNPs. Long-term, this research is expected to generate novel therapeutic and diagnostic tools that can be used for targeted drug delivery and biomedical imaging.

Age-related neuronal changes, lifespan pathways and maintenance of neuronal architecture

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The age-dependency of cognitive decline is well-known in humans, however the mechanisms by which nervous system dysfunction is triggered during aging are poorly understood. Previous studies have reported age-related neuronal morphological changes in *C. elegans.* We have expanded this analysis with a systematic survey of age-related neuronal changes and find that neuron-type specific structural alterations occur across the entire nervous system during normal aging. Furthermore, our neuroanatomical analysis of long-lived mutants reveals that neuronal morphological alterations can be robustly delayed in some long-lived mutants, but not all, indicating that delayed age-related neuronal change is not always coupled with lifespan extension, consistent with findings on healthspan analysis. We are dissecting the molecular pathways responsible for delaying age-related neuronal alterations in long-lived mutants and their interplay with neuronal maintenance molecules. Our findings indicate that the interaction between molecular mechanisms dedicated to the lifelong maintenance of neuronal architecture and lifespan determination are key to neuronal aging. Given the conservation between the human and *C. elegans* genomes, and in neuronal processes, the genes that protect from or promote neuronal decline in *C. elegans* will advance our knowledge of the principles underlying neuronal maintenance and aging.

Cellular senescence impairs microtubule dynamics in intestinal epithelial cells

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Background. The rise in senescent cells during aging compromises the proper functioning of intestinal epithelia, a common aging-associated health problem. Here, we used butyrate and lopinavir to induce senescence in intestinal epithelial cells (IECs). Butyrate is a common product of the gut microbiome and is also introduced into the intestine through diet. Lopinavir is applied in the clinic as a HIV protease inhibitor.

Methods. The proliferation and nuclear morphology of IECs, as well as the activity of senescence-associated β galactosidase (SA-β-Gal) were assessed as biomarkers of cellular senescence. Microtubule stability was evaluated by testing the resistance to nocodazole. To identify the mechanisms underlying microtubule stabilization, α-tubulin acetylation on lysine-40 (K40), histone deacetylase 6 (HDAC6, deacetylates K40), and several microtubule-associated proteins (MAPs) were monitored by Western blotting and immunofluorescence staining.

Results. Both butyrate and lopinavir successfully induced senescence in IECs. Microtubules in senescent IECs were resistant to nocodazole treatment. While the acetylation of α-tubulin on K40 was upregulated with butyrate; this was not observed for lopinavir. HDAC6 levels decreased upon butyrate treatment, but increased with lopinavir.

Conclusions. This study defines microtubule stabilization as a senescence marker. Both butyrate and lopinavir lead to microtubule stabilization in IECs, albeit through different cellular pathways.

The role of RNA decay and stability in dendritic spines development

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Neurons communicate via synapses that often located at dendritic spines. Central to learning and memory, the highly dynamic nature of spines suggests that gene expression is finely controlled during their development. However, the mechanisms of such control are poorly understood. We thus aim to elucidate the role of mRNA stability in neuronal development in vivo, using the model organism *C. elegans*. The DD-type GABAergic neurons of the worm constitute an excellent model for studying dendritic spines: they form in larvae and mutants affecting their development are available. Since the degradation of mRNAs takes place mainly in ribonucleoprotein granules (RNPs), we will assess the relationship between the regulation of mRNAs in these granules and dendritic spines development. For this, we are building tools to visualize granules in GABAergic neurons to study their spatiotemporal dynamics (number, location and transport) in neurites and near dendritic spines. We are also preparing transcriptomic profiling analyzes of neurons to identify and quantify the types of mRNA deregulated by mutants affecting mRNA degradation. Study the impact of mRNA regulation on neuronal development may contribute to research on the neuronal plasticity and memory.

JunB and Fra2 of the AP-1 transcription factors can regulate the expression of cadherin 3 in testicular Sertoli cells

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In the testis, cadherins(Cdh) are important proteins in the formation of adherent junctions in the blood-testis barrier between Sertoli cells. Aberrant expression of these proteins can interfere with the normal development and differentiation of germ cells, which can lead to reduced fertility. In Sertoli cells, Cdh3 and the transcription factors of the AP-1 family are highly expressed. Our project aims to characterize the transcriptional mechanisms regulating the expression of *Cdh3* by the AP-1 family in Sertoli cells. The AP-1 factors and regulatory elements on *Cdh3* promoter were identified using luciferase reporter assay and ChIP assay in the Sertoli cell lines TM4 and 15P-1. Then, these cell lines were treated with forskolin, an adenylate cyclase activator that can activate AP-1 factors by PKA, to evaluate changes in Cdh3 expression. The results showed that JunB and Fra2 can cooperate to activate *Cdh3* promoter and the regulatory element is located in the proximal region of the *Cdh3* promoter (-144 to +14 bp). Forskolin-treated 15P-1 cells showed an increased

JunB expression and a decreased Cdh3 expression in Western Blot. In conclusion, Jun and Fra2 can cooperate to regulate Cdh3 expression through the recruitement of the hetero-dimers JunB/Fra2 to the proximal region of *Cdh3* promoter.

Mechanisms of maintenance of nervous system architecture: role of the sax-7/L1CAM gene.
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After birth, the organization of the nervous system is maintained despite body growth, loss and addition of neurons, mechanical stress, and aging. Errors in the long-term maintenance of neuronal architecture can lead to neurodegenerative diseases; however, its mechanistic bases are poorly understood. This project aims to better understand the cellular and molecular mechanisms mediated by L1CAM proteins during neuronal post-natal maturation. We use the microscopic worm C. elegans, a powerful model for genetic and molecular studies to decipher universal mechanisms. The worm homolog of L1CAM is SAX-7, which is required for the maintenance of neuronal organization in worms. L1CAM is also required post-developmentally in mice to maintain brain function throughout life, as the conditional depletion of L1CAM in the brain of adult mice results in behavioral deficits. SAX-7/L1CAM is a highly conserved transmembrane protein, whose extracellular region enables interactions with adjacent cells (via immunoglobulin domains), and its intracellular region interacts with the cytoskeleton. We are dissecting the structure-function relationship of SAX-7 and its role via glial cells in long-term neuronal protection. This work will provide information that may contribute to the development of strategies for the detection and treatment of patients with CRASH syndrome or neurodegenerative disorders.

Regulation of m6a related proteins during whole-body freezing of the wood frog, Rana sylvatica
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Freeze tolerance is a known survival strategy used by various amphibians and reptiles, including the freeze-tolerant wood frog, *Rana sylvatica*. The wood frog is one of the few vertebrae organisms that may spend weeks to months with up to 70% of total body water frozen as extracellular ice, showing no physiological vital signs of life, but returning to normal upon thawing. Given that wood frogs require carbohydrate metabolism while frozen, it is reasonable to believe there are regulatory pathways that assist in surviving its frozen state, such as the involvement of m^6A mRNA methylation. In liver tissue, a greater number of mRNA transcripts were methylated in frozen, 3.33-fold, and more so when thawed, 4-fold, then controls. Transcription of m^6A related proteins that methylate mRNA such as METTL14 and WTAP were increased by 1.28-fold and 1.42-fold respectively. The demethylase FTO was notably downregulated by 39% from control levels. Translation activators or proteins in their complexes, such as eIF3a, saw reduced transcription of 64%, and mRNA degraders YTHDF2 and YTHDC2 saw a similar trend decreasing 42% and 22% in freezing. Our results demonstrate that m^6A methylation and proteins implicated in its pathway assist in regulation of metabolism during freezing.

Mechanisms regulating the extracellular matrix to ensure the long-term maintenance of neuronal organization and connectivity

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The function of the nervous system is closely linked to its structure and inter-neuronal connections. Established during embryogenesis, the initial organization of the nervous system must be subsequently maintained, despite the growth of the organism, the integration of new neurons, mechanical stresses related to body movements, accidents, and aging. However, the mechanisms that ensure the protection of the nervous system throughout our lives remain poorly understood. Our research aims to elucidate the mechanisms that ensure the maintenance of nervous system organization and neuronal connectivity throughout life. The nematode *C. elegans* is a powerful model organism with a well-described nervous system enabling to uncover universal principles of neural maintenance that are conserved up to humans. Our previous work demonstrates that interactions between neurons and the extracellular matrix are part of the maintenance mechanism of neuronal architecture. Using molecular genetic approaches (mutant combinations, RNAi, visualization of fluorescently tagged proteins in vivo, etc.), we are evaluating the interactions between extracellular matrix components and modulators, as well as their impact on neuronal and synaptic organization. On the long term, our work will help to understand the bases of some neurodegenerative diseases and will contribute to develop diagnostic/therapeutic strategies.

Developing novel glycan binding proteins for tumor associated carbohydrate antigens by directed evolution

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Sugars coat the cells of each and every living organism, and the complex carbohydrates on the surface of these cells are important for a wide range or interactions in biology. Abnormal sugar patterns on cell surfaces are a hallmark of cancer. One method for diagnosing and treating cancers is based on the identification and the specific binding of these sugars (i.e. carbohydrates or glycans). Recently, developments in the field have identified new cancer sugar profiles that can be targeted by diagnostics or therapeutics. However, there is a lack of binding-proteins designed to target these profiles and no effective method of producing these proteins for new sugar targets. We propose the use of a new binding-protein scaffold in combination with directed evolution to produce glycan binding proteins. The protein scaffold is based on designed ankyrin repeat proteins (DARPins) — small binding proteins engineered to have high binding affinities. Directed evolution and selection by mRNA display can reduce the time to produce binding-proteins from months/years to weeks. Our aim is not only to create novel cancer-targeting proteins, but to provide a framework to accelerate the discovery and production of future proteins for use in cancer diagnostics and therapeutics.

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The CBGRC Organizing Committee

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Le Comité Organisateur de la CRCSCB

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