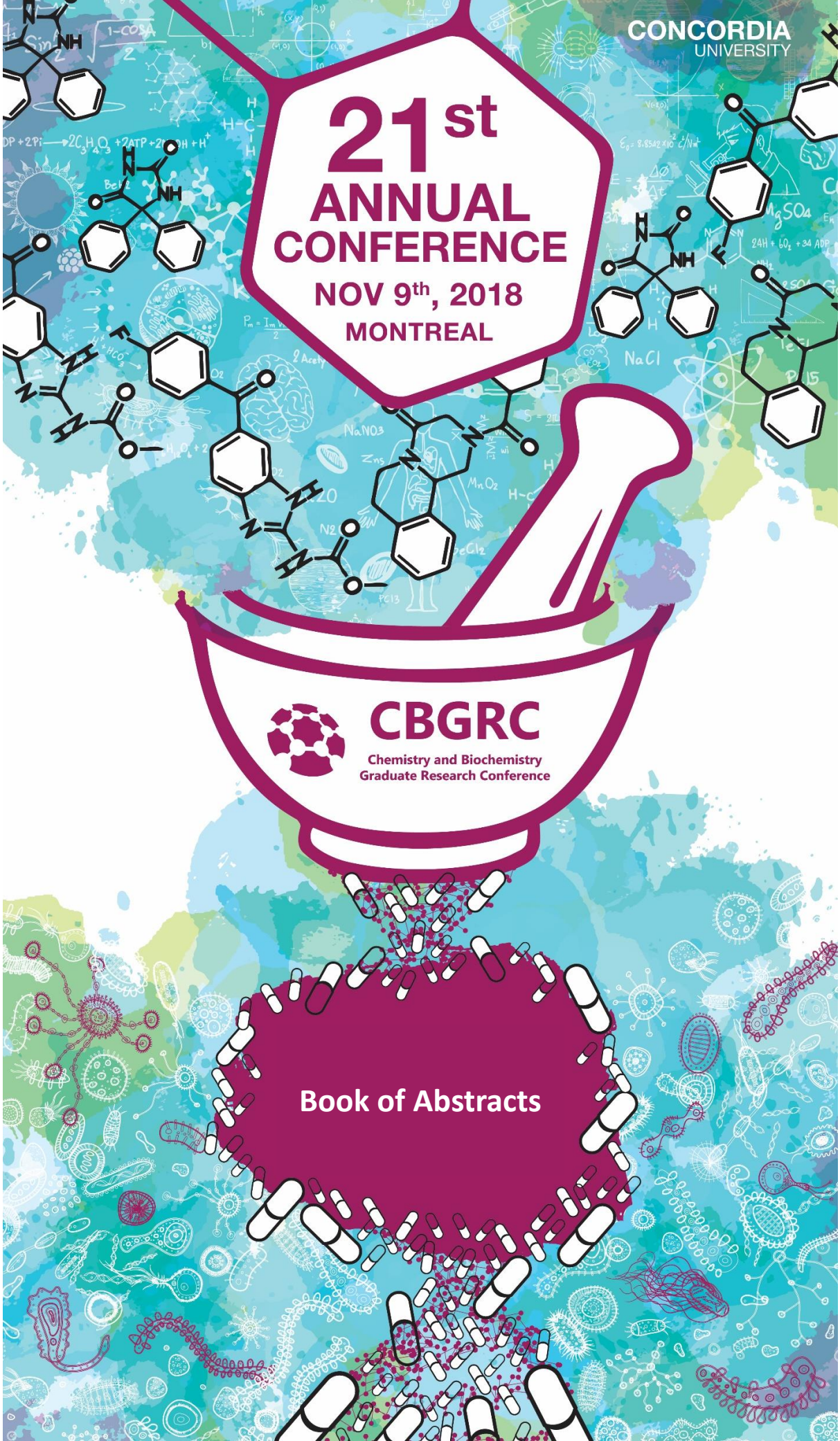
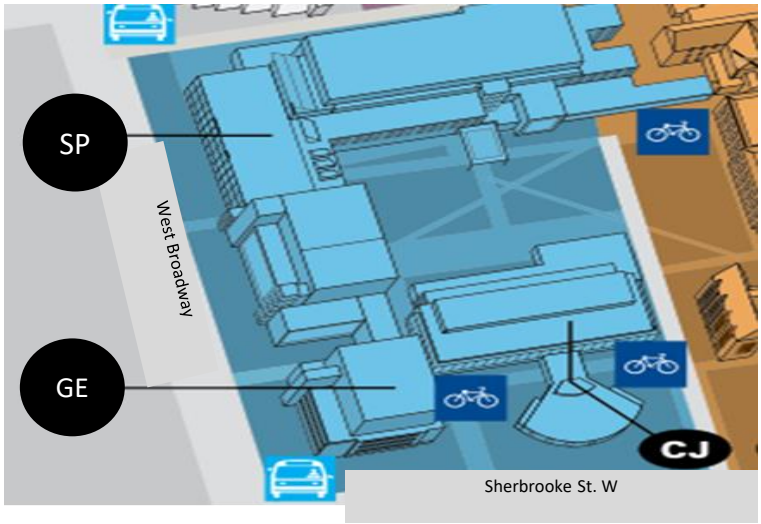

CONCORDIA
UNIVERSITY
21st
ANNUAL
CONFERENCE
NOV 9th, 2018
MONTREAL
CBGRC
Chemistry and Biochemistry
Graduate Research Conference
Book of Abstracts

TABLE OF CONTENTS / TABLES DES MATIÈRES

CAMPUS MAP
PLAN DU CAMPUS

BULDINGS

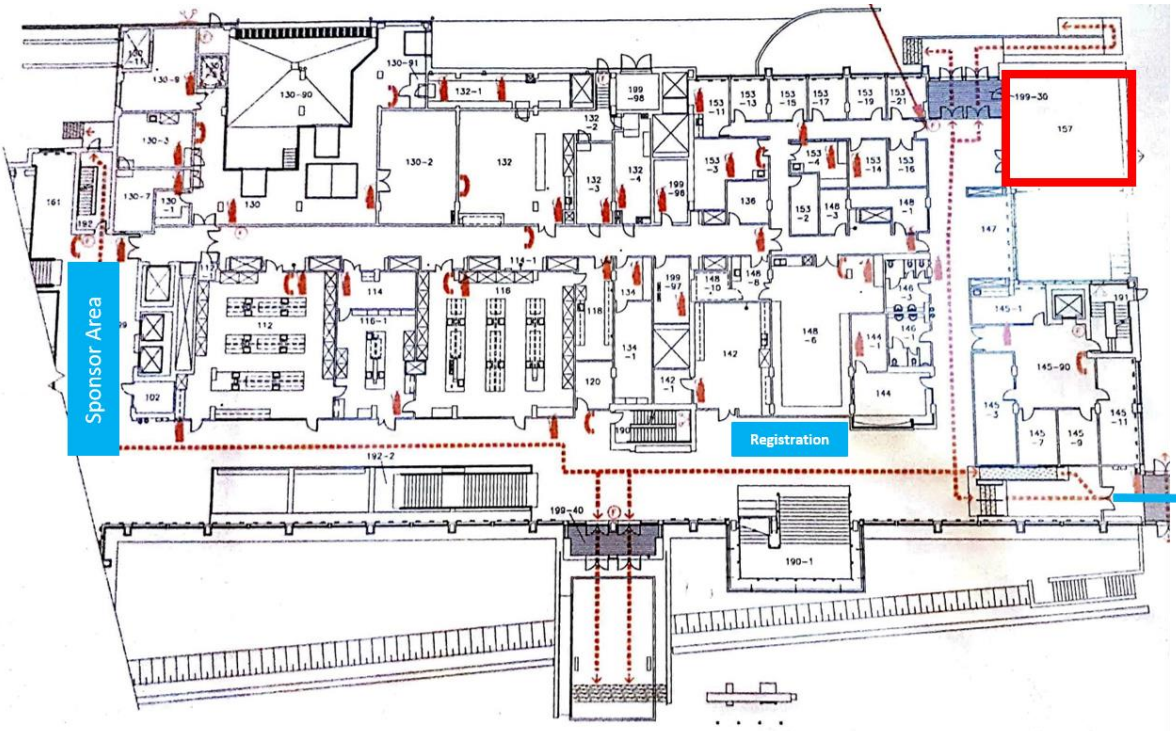


ELEVATORS

STAIRS

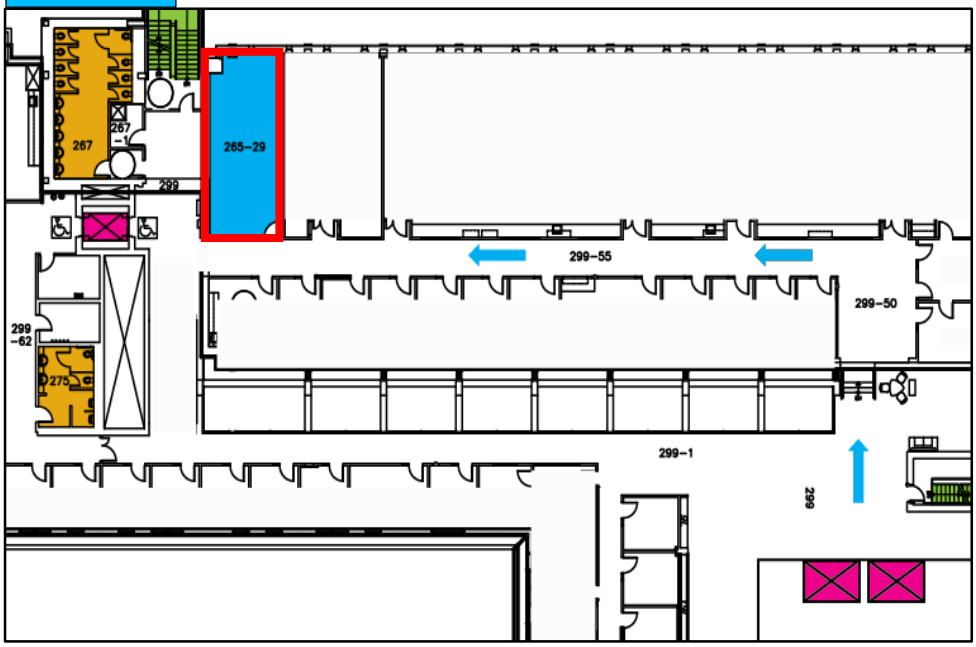
WASHROOMS

SP 1st Floor



CAMPUS MAP
PLAN DU CAMPUS

SP 265.29



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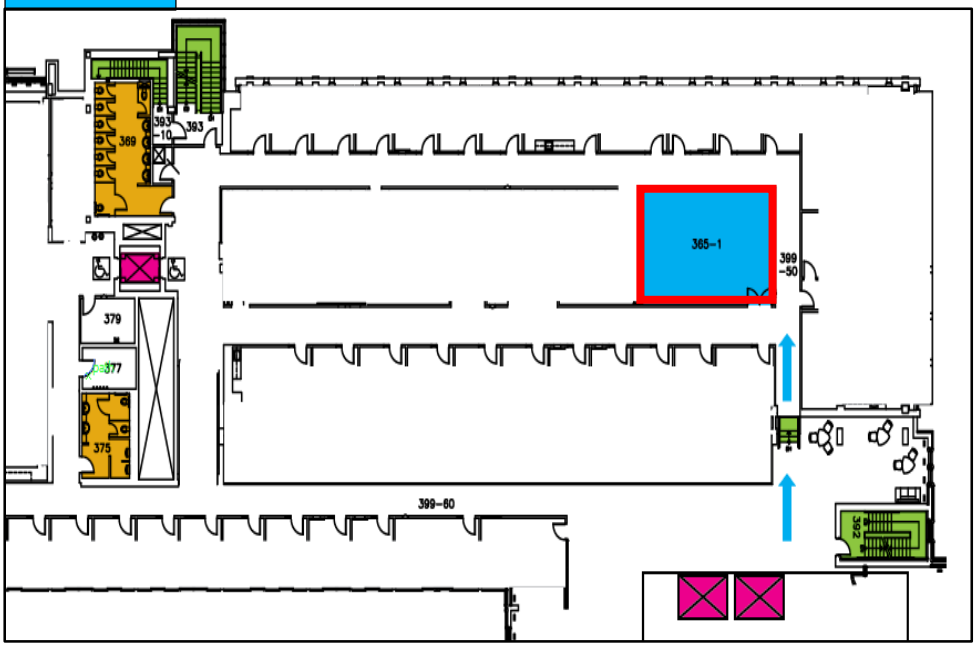


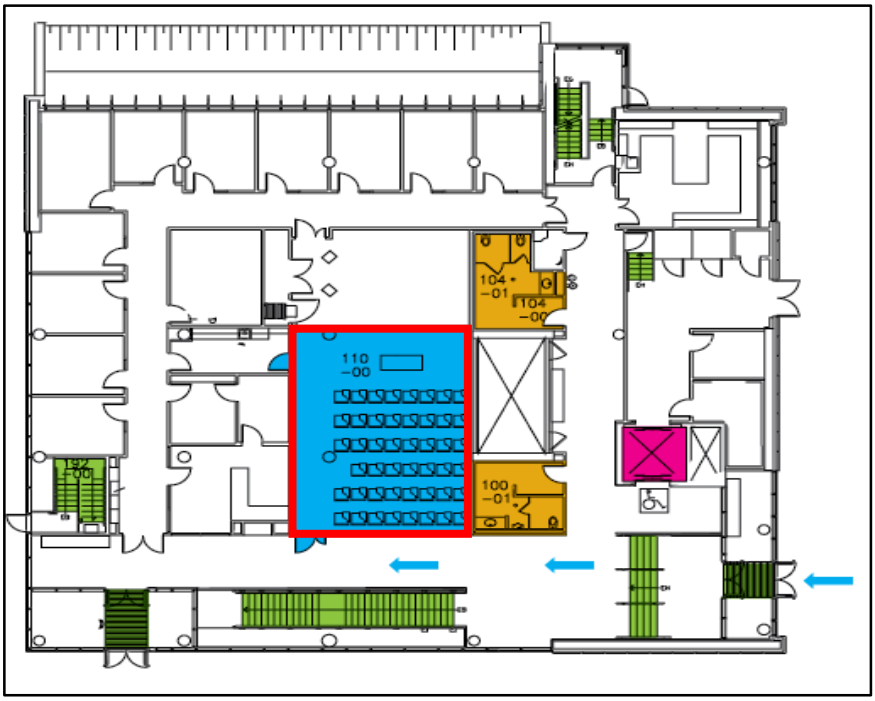
ELEVATORS

STAIRS

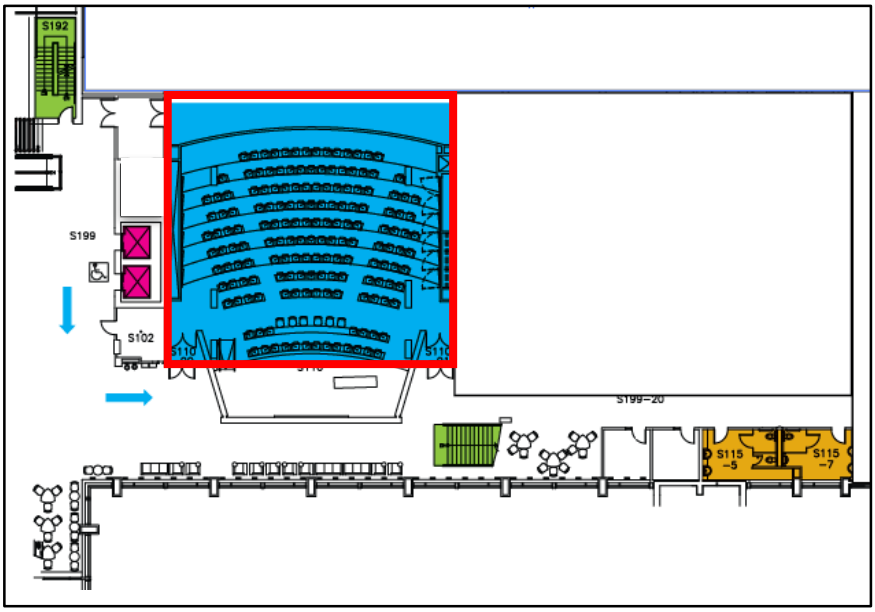
WASHROOMS

CAMPUS MAP
PLAN DU CAMPUS

KEYNOTE SPEAKER 1 GE 11-.00



KEYNOTE SPEAKER 2 SP S-110.00



ELEVATORS

STAIRS

WASHROOMS

WELCOME NOTE
LETTRE DE BIENVENUE

Dear friends and colleagues,

It is with great pleasure that we welcome you all to the 21st annual Chemistry and Biochemistry Graduate Research Conference. This year, we are especially proud to host such a diverse conference. With a wide range of topics, the keynote and graduate presentations are sure to be stimulating and made even better by the participation of various participants and judges. The organizing committee has provided the best environment for graduate students, professors and industry representatives to share and discuss their research and build new connections. We hope this conference will be productive and inspiring to all!

Once again, we would like to extend our gratitude to you all for contributing to the CBGRC this year.

The CBGRC Organizing Committee

Chers amis et collègues,

C'est avec un immense plaisir que nous vous accueillons à la 21ième Conférence sur la recherche aux cycles supérieurs en Chimie et Biochimie. Cette année, nous sommes particulièrement fiers de vous accueillir à une conférence d'une telle diversité. Les conférenciers invités ainsi que les étudiants aux cycles supérieurs vont vous stimuler en présentant un éventail de sujets abordés; améliorés par l'appui des participants et des juges. Le comité organisateur a fait de son mieux pour fournir aux étudiants, professeurs et représentants de l'industrie le meilleur environnement possible pour partager leur recherche et bâtir de nouvelles collaborations. Nous espérons que cette conférence sera productive et inspirante pour tous!! De nouveau, nous tenons à exprimer notre gratitude envers vous tous pour votre participation à la CRCSCB cette année.

Le Comité Organisateur de la CRCSCB

MORNING KEYNOTE SPEAKER
INTERVENANTS PRINCIPAUX

Dr. Timothy Geary

Canada Research Chair in Parasite Biotechnology; Institute Director

Faculty of Agricultural and Environmental Sciences

McGill University

Drug Discovery for Neglected Tropical Diseases: Reversing the Equation

Infections of humans by parasitic helminths once were global in incidence. More than a billion people still serve as hosts to these worms, almost all of them living in developing nations. These Neglected Tropical Diseases cause significant morbidity, contributing to the cycle of poverty which constrains development in resource-limited regions. Medicines to treat these infections have generally been adopted from veterinary use (for livestock and companion animals) and have not been optimized for humans. Several are donated by Western pharmaceutical companies for use in humans in Africa and elsewhere. An alternative approach is to foster innovation systems that enable scientists living in areas most affected by these diseases to assume leadership roles in the search for new and better medicines to treat them.

This lecture introduces parasitic diseases of poverty and describes a novel drug discovery process that was implemented in South Africa and Botswana, focused on identifying high-value antiparasitic drug candidates in collections of chemicals purified from African sources. Changing the way in which drugs are provided to regions of poverty requires the strengthening of scientific capacity as well as the development of new ways of thinking about intellectual property and the requirement for local leadership. Integrating multiple levels of drug discovery and development in this context is an unfinished story with significant challenges and great potential.

Dr. Tomislav Friščić
Associate Professor
Department of Chemistry,
McGill University

Chemistry 2.0

Rapid consumption of feedstocks, coupled with a massive impact of chemical manufacturing on the environment, has greatly increased the interest and awareness of chemists in the development of cleaner, safer and more efficient chemical methodologies. A major concern are solvents, that are globally used in excess of 30 million tons and largely end in toxic waste. As chemistry is unimaginable without solvents, addressing this problem requires a re-examination of a fundamental principle of how chemistry is performed. Over the past decade mechanochemistry, *i.e.* reactions induced by milling or grinding,[1] has been applied with great success to a wide range of systems, from organic and inorganic synthesis, to organometallics, functional materials (metal-organic frameworks, pharmaceutical cocrystals) and nanomaterials.

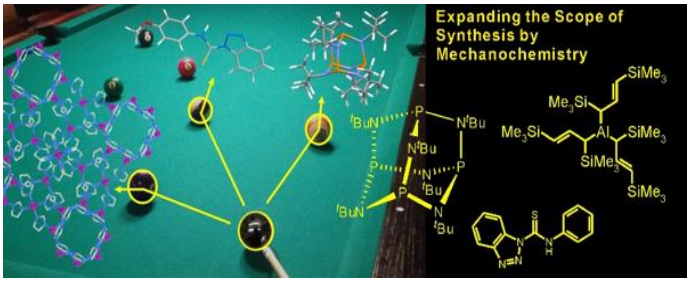


Image: Jean-Louis Do, Concordia University and McGill University

While mechanochemistry offers a general route to conduct chemistry without bulk solvents, it also provides a means to discover reactions and synthesize targets that are difficult or even considered impossible to make from solution. It appears that mechanochemistry and related solvent-free methods could provide access to *Chemistry 2.0:* the cleaner, safer and more efficient chemistry sought by modern chemists.[2]

1. Do, Friščić *ACS Centr. Sci.* **2017**, *3*, 13.
2. Do, Friščić *Synlett.* **2017**, *28*, 2066.

SCHEDULE
HORAIRE

TIME	EVENT	Location
08:00 - 19:00	Registration (All Day)	SP Building Security Station
08:00 - 09:15	Breakfast	SP Atrium
09:15 - 10:15	**Student Presentation A**	**Analytical Chemistry (SP-265.29)** **Molecular Biology (SP-365.01)** **Organic Chemistry (SP-244.09)**
10:15 - 10:45	Coffee Break and Sponsors Exhibition	SP Atrium
10:45 - 11:45	**Keynote Speaker – Dr. Timothy Geary**	**GE-110**
11:45 - 13:00	Lunch and Sponsors Exhibition	SP Atrium
13:00 - 14:30	**Student Presentation B**	**Analytical Chemistry (SP-265.29)** **Computational Chemistry and Nanochemistry (SP-365.01)** **Biochemistry (SP-244.09)**
14:30 – 14:45	Coffee Break and Sponsors Exhibition	SP Atrium
14:45 - 15:45	**Keynote Speaker – Dr. Tomislav Friščić**	**SP-S110**
15:45 - 17:30	**Student Presentation C**	**Organic Chemistry (SP-265.29)** **Molecular Biology (SP-365.01)** **Biochemistry (SP-244.09)** **Inorganic Chemistry and Physical Chemistry (SP-157)**
17:30 - 19:30	**Poster Presentations**	**Jesuit Hall - RF-130**
17:30 - 22:00	Wine & cheese	**Jesuit Hall – RF 100**

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

(SP 265.29)

(9:15) M. Sansoucy (Université du Québec à Montréal): Comparison of Reverse Phase Fractionation Approaches for 2D-LC-MS/MS Analysis of Liver Proteins

(9:30) Y. Pan (McGill University): Investigation of Silver Nanoring as An Electrocatalyst

(9:45) M.-P. Ouellet (Université de Montréal): Improvement of Robustness and Enzymatic Activity of Reticulated Proteolytic Enzymes with Glutaraldehyde for Peptide Mapping by Capillary Electrophoresis

(10:00) F. Leone (Concordia University): Analysis of the $^{13}C/^{12}C$ Ratio of Bacteria-Specific Fatty Acids to Determine the Lability of Terrestrial and Marine Organic Matter in Sediment of the St.-Lawrence Estuary and Gulf.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

(SP 365.01)

(9:15) N. Zamorano (CRCHUM - Université de Montréal): Enrichment of Oxidized Peptides Allows Identification of Oxidized Cysteine Residues in Signaling Proteins *In Vivo*

(9:30) C. Li (Institute for Research in Immunology and Cancer - Université de Montréal): Quantitative Proteomics Identifies Novel PIAS1 Protein Substrates Involved in Cell Migration and Motility

(9:45) L. Miller (University of New Brunswick): The Role of the Retrotransposon I-Element Protein ORF1p in Retroduplication in *Drosophila*: RNA Binding in the Female Germline

(10:00) B. Pakseresht (Concordia University): Isolation and Characterization of Marine Myxobacteria

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

(SP 244.09)

(9:15) J. Stille (McGill University): Computationally-Aided Design and Synthesis of Inhibitors of Activation-Induced Cytidine Deaminase for the Treatment of Leukemia and Lymphoma

(9:30) S. Ricard (Université du Québec à Montréal and UQTR): Synthesis of γ,δ-Unsaturated α-Aminoketones Using a Tandem Copper-Catalyzed Vinylation Reaction Followed by a Claisen Rearrangement

(9:45) B. Keenan (McGill University): Reconstructing Human Population Dynamics in the Southwestern Maya Lowlands from a Tropical Lake Core

(10:00) N. Truong (University of Alberta): Predictable Cleavage of Unsymmetrical Dialkyl Ethers

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

(SP 265.29)

(13:00) B. Desharnais (Concordia University): Tackling Endogenous Concentration in Production Operations *via* an Automated R Script: Application to BHB analysis

(13:15) B. Garneau (Université du Québec à Trois-Rivières): Development of a Screening Method for Novel Synthetic Opioids Using a DOE Approach and Application to Casework

(13:30) S. Pfammatter (IRIC - Universite de Montreal): Enhanced Immunopeptidome Identification and Quantitation with High-Field Asymmetric Waveform Ion Mobility (FAIMS) Combined with TMT-Labeling.

(13:45) V. Prinville (Université du Québec à Montréal): Quantitative Method to Analyze the Effect of Acetaminophen on Bile Acids in Rat Plasma by LC-MRM

(14:00) I. Slobodchikova (Concordia University): Characterization of Human Mycotoxin Metabolites Using Microsomal Incubations and Mass Spectrometry

COMPUTATIONAL CHEMISTRY/CHIMIE NUMÉRIQUE & NANOCHEMISTRY/NANOCHIMIE

(SP 365.01)

(13:00) H. Hu (Concordia University): Molecular Simulation of Metalloid and Group 14 Nitride's Mechanical and Electrical Properties

(13:15) B. Metneja (Concordia University): Computational Exploration of Reaction Pathways

(13:30) F. Charih (Carleton University): MethylSight: A Computational Approach to the Elucidation of the Methyllysine Proteome

(13:45) M. Arhangelskis (Department of Chemistry, McGill University): Prediction of Topological Preferences and Energetic Properties of Metal Azolate Frameworks Using Periodic DFT Calculations

(14:00) Z. Pei (University of British Columbia): Study of Radical Clock Reactions with High-level Computational Technique

(14:15) A. Auge (Université de Sherbrooke): Nanogels UCST à Base de Poly(acrylamide-co-acrylonitrile) Réticulés par un Colorant à Base de Nickel Bis(dithiolène) Capable d'Absorber dans le Proche Infrarouge et Évaluation de leur Efficacité Photothermique

BIOCHEMISTRY/BIOCHIMIE

(SP 244.09)

(13:00) R. Collins (Carleton University): Non-Histone Substrates for Histone Methyltransferases: Investigating MLL4-Dependant Methylation of 53BP1 and Cfp1

(13:15) J. Porro Suardiaz (Concordia University): Interaction of Bacterial and Cancer Cells Model Membranes with GL13K: An Antimicrobial Peptide with Anticancer Activity

(13:30) C. Rinfret Robert (Université de Montréal): Regulation of SUMOylation, Phosphorylation
and Ubiquitination in Response to Arsenic Trioxyde, a Therapeutic Agent Used in the Treatment of Acute Promyelocytic Leukemia

(13:45) A. Poulhazan (Université du Québec à Montréal): Using Solid-State NMR to Fully Assign Starch Chemical Shifts: Purified and In-Cell Carbohydrate Polymer Characterization

(14:00) L. Zaroubi (Concordia University): The Investigation of the Chemical Ecology of Geosmin

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

(SP 265.29)

(15:45) F. Chacon-Huete (Concordia University): Environmentally Benign Reactions on Biomass-Derived Furans as a New Strategy for the Synthesis of Complex Value-Added Materials

(16:00) C. Messina (Concordia University): Sequential Palladium-Catalyzed Decarboxylative Cross-Couplings for the Facile Synthesis of Non-Symmetic Arylated Thiophene

(16:15) C. Buonomano (Concordia University) Synthesis of Tunable Anion Receptors using Palladium-Catalyzed Decarboxylative Cross-Coupling Reactions

(16:30) J. T. Liu (Concordia University): Utilizing Decarboxylative Cross-Coupling for a Discrete Library of Oligothiophene

(16:45) A. Dominguez-Huerta (McGill University): Catalytic *N*-Modification of a-Amino Acids and Small Peptides with Phenol under Bio-Compatible Conditions

(17:00) M. Cloutier (Institut national de la recherche scientifique - Institut Armand-Frappier): *Burkholderia Pseudomallei* and *Burkholderia Mallei* Synthetic Lipopolysaccharide Mimics as Potential Vaccine Candidates

(17:15) S. Pinus (McGill University): Computational Design and Synthesis of Asymmetric Catalysts

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

(SP 365.01)

(15:45) H. Moteshareie (Carleton University): Heavy Metal Sensitivities of Gene Deletion Strains for *ITT1* and *RPS1A* Connect their Activities to the Expression of *URE2*, a Key Gene Involved in Metal Detoxification in Yeast

(16:00) I. Nad (University of Ottawa): Molecular Control of Genome Architecture

(16:15) D. Hossain (McGill University): The Role of NPHP5 in Basal Feet Formation

(16:30) A. Heidari (Western University): Synthesis of 2-thiouracil PNA Monomer for Fmoc-Based Synthesis of Pseudo-Complementary Oligomers

(16:45) H. Hadj-Moussa (Carleton University): Genes of the Undead: Do Hibernators and Zombies Display Similar Expression Profiles

(17:00) D. Duncan (McGill University): Resensitization of *Salmonella Enterica* Ser. Typhimurium to the Macrophage Metabolite Itaconate *In Vitro* and *In Cellulo*

(17:15) H. Bo (Carleton University): Role of Oxygen on Nuclear Factor Erythroid-2-like 1 (NFE2L1) Function and Stability

BIOCHEMISTRY/BIOCHIMIE

(SP 244.09)

(15:45) A. de Aguiar Lopes (Concordia University): Maturation of Heme Proteins in *Saccharomyces cerevisiae*

(16:00) S. Dastpeyman (Concordia University): Visualizing the Heme Status of a Protein Using Green Fluorescent Protein

(16:15) M. Hoekstra (Carleton University): Development of Enzyme Activity Assay to Study Substrate Selection of KDM5/JARID1 Family of Lysine-Specific Histone Demethylases

(16:30) G. Park (Western University): A Chimeric Nucleobase - Phenylazo Derivative as an Intrinsic Nucleobase Quencher

INORGANIC CHEMISTRY/CHIMIE MINÉRALE & PHYSICAL CHEMISTRY/PHYSICO-CHIMIE (SP 157)

(15:45) F. Akogun (University of Otago): Carbazole-Based Complexes as Catalysts

(16:00) O. Schott (Université de Montréal): High Photocatalytic Efficiency of Molecular Ru-Co System for Solar Fuel Generation

(16:15) A. Bain (McGill University): Overcoming the Barriers to Characterizing Strongly Absorbing Aerosol Particles

(16:30) B. Guzman (McGill University): Detection of Nanoscale Phase Separation in Nanoparticles with Mixed Ligand Shells by Solid State NMR

(16:45) H. Hase (Department of Physics, Concordia University, Montreal, Canada): Unraveling the Microstructure of Molecularly Doped P3HT by Thermally-Induced De-Doping

(17:00) B. Wallace (McGill University): Aerosol Diffusivity Studies: Single-Particle Experiments Using Optical Traps

POSTER SESSION
17:30-19:30 RF-130

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

A01 - L. Dupont (Concordia University): Detection of Crude Oil Contamination using n-Alkane and PAH Diagnostic Ratios

A02 - T. Geib (Université du Québec à Montréal): Identification of Acetaminophen-Related Covalent Protein Binding to Glutathione *S*-Transferase by LC-MS/MS

A03 - A. Guesmi (Université du Québec à Montréal): Studying the Metabolism of Sunscreen Compounds *In Vitro* Using LC-MS/MS

A04 - A. Kormendi (Concordia University, GEOTOP): Stable-Carbon Isotope Analysis of Carbon Redox End-Members Within Hypoxic Estuarine Sediments

A05 - M. Lépine (Université du Québec à Montréal): Determining Isocyanate Exposure in Human Urine by LC-MRM

A06 - O. Ousji (Université du Québec à Montréal): *In Vitro* Oxidative Metabolism and GSH Adduct Formation of Bisphenol A Analogs by LC-MS/MS

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

I01 - T. Bossé-Demers (Laval University): Études de Triaryles Boranes dans le But d'Utilisation pour des Batteries de Types « Redox-Flow »

I02 - N. Bouchard (Université Laval): N-B Bifunctionalized Polystyrene Resins as Recyclable Pre-Catalysts for the Metal-Free Borylation of Heteroarenes

I03 - J. J. Castro (Université de Montréal): Boron Complexes of *N,N'*-Diphenylbenzamidine-*N*-Oxide Ligands with Crystallization-Induced Emission Enhancement Characteristics - Towards Blue and White OLED Applications

I04 - G. Golbaghi (INRS-Institut Armand-Frappier): Ruthenium Complexes of Anastrozole as Potential Multitargeting Chemotherapeutic Agents

I05 - C. Lennox (McGill University): Isolation of Imidazolate Borate Building Blocks and their Mechanochemical Conversion to Ultralight Imidazolate Frameworks

I06 - S. Li (McGill University): Solid-State Routes to the Mixed-Metal Organic Mineral Paceite and its Synthetic Cadmium Analogue

I07 - E. Rochette (Université Laval): Synthesis and Reactivity of Amino-Hydroborane Frustrated Lewis Pairs

I08 - H. Saavedra-Lavoie (Université de Montréal): Synthesis and Characterization of a Family of $Al(AMOX)_3$ Aluminum Complexes

I09 - O. Schott (Université de Montréal): Molecular Photo-Electro Catalytic System for Hydrogen Generation

I10 - H. M. Titi (McGill University): Hypergolic Metal-Organic Frameworks as a New Class of Greener Hypergolic Fuels

I11 - R. Vidal (INRS-Institut Armand-Frappier): Development of Antibiotics that are Highly Selective for N. Meningitdis and N. Gonorrhoeae

I12 – H. Singh (Concordia University): Partial Hydrogenation of Nitro to Hydroxylamine Group in Multidentate ligands

POSTER SESSION
17:30-19:30 RF-130

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

P01 - A. Al Ahmad (Université de Montréal): Component Exchange for Property Tailoring

P02 - J. Gaba (Concordia University): Computational Study of Weak Interactions in Cyclic and pi-stacked Arrangements of Model Phenolic Surfactants

P03 - Z. Kara Ali (Université de Montréal): Phenyl vs. Cyclohexyl Ancillary Groups in Aminotriazine Molecular Glasses: Effect on Interaction Availability and Glass-Forming Ability

P04 - M. Lerond (Polytechnique Montreal): ProDOT Derivatives: Towards Stretchable Organic Electronics

P05 - L. Sant Anna Pereira (Concordia University): Photo-oxidation of Langmuir Monolayers Mediated by the Hypericin Photosensitizer

P06 - J. Vainauskas (McGill University): Engineering Dichroic Cocrystals Using Halogen Bonds

P07 - C. Yao (Université de Montréal): Pushing the Visible Emission Envelop: Developing NIR Emitters

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

O01 - C. Buonomano (Concordia University): Heteroaromatics Synthesis by Decarboxylative and Desulfinative Palladium-Catalyzed Cross-Coupling Reactions using Continuous-Flow Chemistry

O02 - A. Malinge (Département de Chimie, Université de Montréal): Synthesis and Characterization of Liquid Crystalline Tetraoxapentacene Derivatives

O03 - K. Muru (Institut National de la Recherche Scientifique-Institut Armand-Frappier): *En route* to Agminosides Synthesis, Natural and Polyacetylated Glycolipids

O04 - A. Pontarelli (Concordia University): Preparation of Alternative Nucleic Acid Structures and Evaluation of their Repair by AGT

O05 - G. Ravicoularamin (Institute Amand Frappier-INRS): Synthesis of Potential Inhibitors of Bacterial Kdo-Processing Enzymes

O06 - A. Shafeii (Concordia University): Identification of a Novel Anti-Cancer Target with Thioenoisoquinoline Derivatives

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

M01 - D. Abou Samhadaneh (McGill University): Lanthanide-doped upconverting nanoparticles induce stress in mammalian cells

M02 - R. Al-attar (Carleton University): GATA4-Mediated Gene Expression Promotes Muscle Remodeling During Stress in the Freeze-Tolerant Wood Frog, *Rana Sylvatica*

M03 - A. F. Cisneros (Laval University): Effect of Binding Interference on the Divergence Between Paralogous Genes Encoding Homodimers

M04 - G. Derevyanko (Concordia University): TorchProteinLibrary

M05 - A. Gupta (Carleton University): OCT Induced Transcriptional Network in the Freeze-Tolerant Wood Frog

M06 - H. A. Jain (Laval University): *In Silico* Study of Epistasis in Protein Protein Interactions

M07 - Z. Lung (Carleton University): Peroxiredoxin Expression in the Wood Frog, *Rana sylvatica* in Response to Freezing

M08 - O. Moujaber (McGill University): Exploring Stress Granule Formation in Senescent Kidney Cells

M09 - P. Prabhala (Universite de Montreal): Study of Localization and Function of Cep44

M10 - K. Storey (Carleton University): Gene Regulation During Hypometabolism - Coping with Environmental Stress

M11 - S. Takalloo (Carleton University): Identification and Investigation of Novel IRES Trans-Acting Factors Found to Nonspecifically Regulate Multiple Eukaryotic IRES Elements

M12 - A. Watts (Carleton University): m6A Methylation Alters Translational Activity during Hibernation in a Small Mammal, the 13-Lined Ground Squirrel.

M13 - N. Zamorano (CRCHUM - Université de Montréal): Enrichment of Oxidized Peptides Allows Identification of Oxidized Cysteine Residues in Signaling Proteins *In Vivo*

NANOCHEMISTRY/NANOCHIMIE

N01 - W. Copp (Concordia University): Influence of Nucleotide Modifications at the C2′ Position on the Hoogsteen Base-Paired Parallel-Stranded Duplex of Poly(A) RNA

N02 - F. Victoria (Concordia University): Residual Chirality in Carbon Dots from Enantiomers of Amino Acids

N03 - F. Yarur Villanueva (Concordia University): Visible-Light Sensitization of Inorganic Semiconducting Nanostructures for Photoelectrochemical Energy Conversion

N04 - Z. Singh (Concordia University): Developing and Integrating Donor Chromophore Acceptor (D-C-A) Assemblies onto Semiconductor Surfaces to Drive Single Electron Transfer Processes

N05 - K. Jeon (University of Toronto Scarborough): Synthese of Polyserotonin Nanoparticles for Anti-Bacterial Applications

POSTER SESSION
17:30-19:30 RF-130

BIOCHEMISTRY/BIOCHIMIE

B01 - A. Boraman (Laurentian University): New Investigation of Mannose Lipid in Peptide Drug Development

B02 - A. Chopra (Carleton University): Quantification of Proteins in Solution *via* Ultraviolet-Induced Reactions of 2,2,2-Trichloroethanol with Tryptophan and Tyrosine Residues

B03 - S. Green (Carleton University): Regulation of the TCA Cycle Through Modification of the α-Ketoglutarate Dehydrogenase Complex in a Mammalian Hibernator, the Richardson's Ground Squirrel (*Urocitellus Richardsonii*)

B04 - T. Nelson (Université de Montréal, Institute for Research in Immunology and Cancer): SUMO Site- and Paralog-Specific Identification by Mass Spectrometry

B05 - R. Randhawa (McGill University, Concordia University): Investigating New Roles for Cytochrome C Peroxidase (Ccp1) in Antioxidant Defense Using its M172a Variant

B06 - A. Saran (McGill University, Concordia University): Biophysical Analysis of Heme Binding to Human Glyceraldehyde-3-Phosphate Dehydrogenase

B07 - G. Singh (Carleton University): Mondo A: A Key Regulator of Sugar-Induced Gene Expression in Frozen Wood Frogs, *Rana Sylvatica*

B08 - K. Szereszewski (Carleton University): Novel Research - Biochemistry and Molecular Biology of Environmental Stress

ENVIRONMENTAL CHEMISTRY/CHIMIE ENVIRONNEMENTALE

E01 - E. Eysseric (Université de Sherbrooke): A Non-Target Workflow for the Identification of Trace Organic Contaminants Using LC-MS/MS

E02 - G. Garwell (McGill University/ Cardiff University): Benign by Design and by Synthesis: Mechanochemical Solvent-Free Synthesis of Edible MOFs

E03 - N. R. Gervasi (Department of Atmospheric and Oceanic Sciences, McGill University): The Development of a Model to Predict the Viscosity of Atmospheric Aerosols

E04 - L. Lahens (Université de Sherbrooke): Study of the Occurrence of Trace Organic Contaminants in Eastern Canadian Lakes

E05 - A. Lapointe (Université de Montréal): Method Development for Trace-Level Quantification of Nitrosamines in Wastewater

E06 - P. A. Segura (Université de Sherbrooke): Removal of Pharmaceuticals in Hospital Wastewaters by Wet-Air Oxidation

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

Comparison of Reverse Phase Fractionation Approaches for 2D-LC-MS/MS Analysis of Liver Proteins

M. Sansoucy*, L. Sleno

UQAM

Liver microsomes and S9 fractions are common *in vitro* model systems for toxicological and pharmaceutical studies. Whole liver homogenates are highly complex and therefore pose additional technical difficulties for comprehensive proteomic analyses. Following enzymatic digestion of proteins, multi-dimensional separation uses orthogonal chromatography techniques, such as ion exchange separation, to online LC-MS/MS. In parallel, reverse phase fractionation has recently been introduced as a complementary method to ion exchange for peptide separation and is thought to be complementary to acidic LC-MS/MS analysis. In this work, we evaluated the ability of high- and low-pH fractionation to pre-fractionate peptides from S9 fractions. The chromatographic separation was optimized (gradient and fractionation window) for a better peptide collection. Fractionated samples were then concatenated to enhance peptide resolution and reduce LC-MS/MS analysis time by half. Future experiments will include a comparison of S9 digests using strong cation exchange fractionation.

Investigation of Silver Nanoring as An Electrocatalyst

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Carbon dioxide is known as a greenhouse gas. Since industrial revolution, the consumption of fossil fuels has led to a rapid increase in CO_2 emission, disrupting the carbon cycle and leading to a global warming impact. Selective electrochemical CO_2 reduction is thought to be a potentially economical route to tranform it into useful chemicals and fuels. We have discovered a silver nanoring material which is able to reduce CO_2 in bicarbonate electrolyte. We use tobacco mosaic virus coat protein (TMVcp) as a command surface to grow and assemble discrete silver nanoring under UV light illumination. Compared to bulk silver and isolate free nanoparticles, the nanoring exhibits an enhanced CO_2 reduction acitvity as well as selectivity towards CO.

Hydrogen evolution reaction is a main route for producing H_2 gas, which is the cleanest and one of the most promising energy carriers. The above silver nanoring shows increased electrocatalytical behavior compared to bulk silver and free nanoparticles in acidic conditions. Computational studies will be needed to understand the fundamental reason of the enhanced performance for both CO_2 reduction and hydrogen evolution by the ring structure.

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

Improvement of Robustness and Enzymatic Activity of Reticulated Proteolytic Enzymes with Glutaraldehyde for Peptide Mapping by Capillary Electrophoresis

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In bottom-up proteomics, an essential technique that is routinely used is enzymatic digestion of proteins. The use of insoluble enzymes offers several benefits such as reusability, high enzyme-to-substrate ratio, which allows rapid digestion and limited autoproteolysis. Our group is using two proteolytic enzymes, trypsin and chymotrypsin, and a crosslinking agent, glutaraldehyde (GA), to immobilize both enzymes. Previous studies showed that reticulated GA-chymotrypsin could only be used for two consecutive digestions due to an apparent de-aggregation of the enzyme particles resulting in loss of enzymatic activity. Further studies were thus needed to investigate the nature of de-aggregation to see if this loss in activity comes from mechanical shearing caused by the rigorous washing steps or from chemical dissociation of the enzyme-GA crosslinks. Therefore, several washing conditions were evaluated as well as different storage conditions (temperature, solvent composition). These investigations were characterized by comparing the peptide maps obtained by capillary electrophoresis with UV-detection (CE-UV) after applying migration time correction between runs achieved using an Igor Pro algorithm based on equations from that describe two-peak normalization of migration times.

Analysis of the $^{13}C/^{12}C$ Ratio of Bacteria-Specific Fatty Acids to Determine the Lability of Terrestrial and Marine Organic Matter in Sediment of the St.-Lawrence Estuary and Gulf.

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Concordia University

Discharge of organic matter (OM) and inorganic nutrients from the St.-Lawrence River into the St.-Lawrence Estuary (SLE) lead to hypoxia (low dissolved oxygen levels,dO_2) in its bottom waters, influencing the health of this ecosystem. Higher primary productivity as a result of increased nutrient levels leads to higher concentrations of dissolved and particulate OM in the water column, resulting in a greater consumption of dO_2 during degradation of OM by microorganisms. To further our understanding of the carbon cycle in the SLE, we will determine the lability of terrestrially-derived and marine OM through the analysis of the $^{13}C/^{12}C$-ratio of bacteria-specific fatty acid (iC15:0,anteiC15:0) using GC-IRMS. We will cultivate ubiquitous bacteria strains responsible for the degradation of OM in marine broth enriched in ^{13}C to assess the relationship and isotopic fractionation between the ^{13}C-signature of the food source and that of the bacteria. Using this calibration and the isotopic signature of the terrestrial and marine OM end-members, we will determine the proportion of OM of each source being degraded along the SLE. A better understanding of the roles of bacteria in the carbon cycle within the St.-Lawrence River will allow improvements in the model describing the dynamics of OM in this system.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Enrichment of Oxidized Peptides Allows Identification of Oxidized Cysteine Residues in Signaling Proteins *In Vivo*

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Detection of oxidative post-translational modifications (ox-PTMs) of Cys residues in mammalian signaling proteins *in vivo* is one of the current challenges in redox biology. Ox-PTM residues labeling using switch methods coupled to mass spectrometry (M/S) or immunoblot have rendered possible the identification of signaling proteins subjected to ox-PTM. However, the low sensitivity remains a major hurdle to the detection of the modified residue(s) for the low abundant less reactive proteins. Here, we report a modified method of ox-PTM protein labeling coupled to M/S that highly improved the enrichment of oxidized peptides and the identification of specific ox-PTM Cys residues *in vivo*. In cell lines treated with diamide, a thiol-oxidizing agent, or HOCl, we identified 2699 peptides, covering 1473 proteins, containing at least 1 ox-PTM Cys residue. Previously reported ox-PTM residues were confirmed *in vivo*, validating our approach. Signaling proteins, including kinases, phosphatases and translation factors are largely represented. Altogether, the use of an improved method with higher sensitivity for the detection of ox-PTM Cys residues *in vivo* allowed us to deepen our understanding of redox signaling. Network analyses allowed us to highlight signaling pathways enriched in oxidized proteins related to innate immunity, antiviral response and inflammation.

Quantitative Proteomics Identifies Novel PIAS1 Protein Substrates Involved in Cell Migration and Motility

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The Protein Inhibitor of Activated STAT 1 (PIAS1) is a SUMO E3 ligase that plays important roles in various cellular pathways, including STAT signaling and p53 pathway. Increasing evidence shows that PIAS1 is overexpressed in various human malignancies. To understand the mechanism of action of PIAS1, we developed a quantitative SUMO proteomic approach to identify potential substrates of PIAS1 in a system-wide manner. Our analyses enabled the profiling of 983 SUMO sites on 544 proteins, of which 177 SUMO sites on 123 proteins were identified as putative PIAS1 substrates. These substrates were found to be involved in different cellular processes, including cytoskeleton dynamics. Further functional studies on Vimentin (Vim), a type III intermediate filament protein involved in cytoskeleton organization and cell motility, revealed that PIAS1 exerts its effects on cell migration and cell invasion through the SUMOylation of Vim at Lys-439 and Lys-445 residues. Vim SUMOylation was necessary for its dynamic assembly, and cells expressing a non-SUMOylatable Vim mutant showed reduced levels of migration and invasion. Our approach not only provides a novel strategy for the identification of SUMO E3 ligase substrates, but also yields valuable biological insights into the unsuspected role of PIAS1 and Vim SUMOylation on cell migration.a

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

The Role of the Retrotransposon I-Element Protein ORF1p in Retroduplication in *Drosophila*: RNA Binding in the Female Germline

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A retrotransposon is a type 1 transposable element that plays an important role in evolution, affecting gene regulation, as it reverse transcribes its own RNA to create a cDNA copy that is inserted in the genome. Retrotransposons also reverse transcribe other RNAs to produce retroduplications. The human L1 retrotransposon is capable of retroduplication; however, how this happens has not been studied in the germline. The L1 ORF2 protein (ORF2p) is a reverse transcriptase and has endonuclease activity, while the ORF1 protein (ORF1p) has RNA binding activity; however, little is known about the RNA binding preference. The transposition of the I-element, a L1-related retrotransposon in *Drosophila* species, has been studied *in vivo*, however nothing is known about the I-element's retroduplication activity. In this study, a cloned *Drosophila teissieri* I-element is used to explore RNA binding of ORF1p *in vivo*. Three transgenic *Drosophila melanogaster* strains were constructed, with one transgenic strain expressing an epitope-tagged ORF1p in the germline and will be used to determine the types of RNA that are associating with ORF1p. The other transgenic fly strains will assess the full I-element clone for its ability to transpose, and to determine if the HA epitope tag in ORF1p affects this retrotransposition.

Isolation and Characterization of Marine Myxobacteria

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Concordia University

Antibiotic resistance has become a major threat to global health. Patients are prone to hospital-acquired infections, which are often antibiotic-resistant. This may lead to prolonged hospitalization or increased rates of mortality. One solution to this problem is the discovery of novel antibiotics from new strains of antibiotic producing bacteria. Myxobacteria are bacterial predators that produce secondary metabolites which can kill their bacterial prey. This key characteristic of myxobacteria makes them a good target for antibiotic discovery. Although terrestrial myxobacteria are well-studied, marine myxobacteria haven't been fully characterized. It has been shown that novel strains can produce new natural products, which has led us to conduct further studies on marine myxobacteria. We were able to isolate a number of strains from the sediment samples collected from the Gulf of Saint Lawrence by our collaborators. The aim of this study is to isolate marine myxobacteria and cultivate them in order to extract the secondary metabolites. We will characterize these secondary metabolites and study their mechanisms of action which can give us insights into routes of antibiotic biosynthesis.

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

Computationally-Aided Design and Synthesis of Inhibitors of Activation-Induced Cytidine Deaminase for the Treatment of Leukemia and Lymphoma

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Leukemia and lymphoma are two related types of blood cancer which currently affect an estimated 65,000 Canadians and account for nearly half of all childhood cancers. This research project aims to target activation-induced cytidine deaminase (AID), a metalloenzyme heavily implicated in the poor disease progression of both lymphoma and leukemia. We utilise computational software created in our lab to discover lead compounds that can act as metalloenzyme inhibitors, and our docking program FITTED has been specifically developed to accurately model metal-ligand interactions. This presentation will discuss the application of our computational software towards the development of AID inhibitors. We have identified two preliminary inhibitors of AID and have used FITTED to analyze their interactions within the enzyme's active site. Based on the predicted binding poses, we can utilise *in silico* combinatorial chemistry to efficiently identify promising inhibitor analogues. Concurrently, synthetic methodology is being developed to prepare both the initial hits and the computationally-designed analogues. While the preliminary hits show moderate bioactivity, the binding poses indicate that they form predominantly weak, electrostatic interactions with the zinc ion present in the active site. To address this, we have also expanded into virtual-screening to identify compounds that form strong, covalent-like interactions with zinc.

Synthesis of γ,δ-Unsaturated α-Aminoketones Using a Tandem Copper-Catalyzed Vinylation Reaction Followed by a Claisen Rearrangement

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Daoust's group developed an efficient method for the preparation of non-natural alpha-amino acids from simple amides by successive C−N and C−O functionalization of trans-1,2-diiodoethene followed by a Claisen rearrangement. In this project, we extended this method to carbamates, non symmetrical vinyl diiodides and various allylic alcohols in order to synthesize highly functionalized allyl vinyl ethers which were then rearranged into gamma,delta-unsaturated alpha-aminoketones with high diastereoselectivities. The optimization of the method, its application to different substrates, and the versatility of beta-nitrogenated vinyl iodides will be presented.

Le groupe de Daoust a développé une méthode efficace pour préparer des acides alpha-aminés non naturels à partir d'amides simples par fonctionnalisation C−N et C−O successive du *trans*-1,2-diiodoéthène, suivie par un réarrangement de Claisen. Dans le présent projet, nous avons étendu cette méthode aux carbamates, aux diiodures vinyliques non symétriques et à divers alcools allyliques dans le but de synthétiser des allyl vinyl éthers hautement fonctionnalisés. Ces derniers ont été ensuite soumis à un réarrangement de Claisen pour obtenir des cétones alpha-aminées gamma,delta-insaturées avec d'excellentes diastéréosélectivités. L'optimisation de la méthode, son application à différents substrats, de même que la polyvalence des iodures vinyliques bêta-iodés seront présentés.

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

Reconstructing Human Population Dynamics in the Southwestern Maya Lowlands from a Tropical Lake Core

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Coprostanol, the main 5β-stanol found in human faeces, is a potential useful proxy for human populations that can be analysed alongside other palaeoenvironmental proxies in lake sediments. I will present initial results of faecal stanol analyses from sediment cores from Laguna Itzan in Guatemala, as a proxy for the population of Itzan, an ancient Maya population centre.

We find variable amounts of faecal stanols throughout the Itzan sediment core, potentially implying changes in human population through time. We see a peak in the coprostanol/cholestanol ratio at about 639 BCE. with lower ratios in later Maya archaeological periods. This is in contrast to archaeological estimates indicating peak local populations during the Late Classic period (~600 to 800 CE). We see evidence for settlement in the area by at least 1350 BCE, which is earlier than has been inferred from archaeological records. These discrepancies will require further exploration, and may indicate that the coprostanol record is influenced by other factors.

These data indicate that faecal stanols could be a powerful tool for tracing human population dynamics in tropical lake watersheds that can be used to complement archaeological datasets, and to link human populations with environmental change.

Predictable Cleavage of Unsymmetrical Dialkyl Ethers

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The cleavage of C−O bonds is an important reaction in organic synthesis, especially in the degradation and transformation of natural compounds. A number of tactics for this transformation have been reported involving the use of acids, bases or transition metals. Among these approaches, boron tribromide is widely used in stoichiometric amounts for this conversion because of its effectiveness under mild conditions and its tolerance towards many functional groups. However, synthetic applications of boron tribromide has been limited to symmetrical dialkyl or aryloxy ethers, perhaps because of unpredictable regioselectivity with other substrates. In contrast, BCl_3 does rapidly forms stable coordination complexes with unactivated ethers under the same conditions. Taking the best properties of BCl_3 and BBr_3 together, we discovered that disproportionation of BBr_3 and BCl_3 followed by reaction with unsymmetrical alkyl ethers can predictably yield dialkoxy boron chlorides, which quickly convert to the corresponding alcohols with high efficiency and regioselectivity. This presentation will outline the detailed study of this reaction including a broad substrate scope.

Tackling Endogenous Concentration in Production Operations *via* an Automated R Script: Application to BHB analysis

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The presence of endogenous substances in biological matrices used for calibration standards and quality controls (QCs) can compromise validation steps and quantitative analyses. Several approaches to overcome this problem have been suggested, but they create serious problems with regards to the accuracy of the analytes or production capacity. We present here a solution that efficiently addresses this problem. The endogenous analyte concentration is estimated via a standard-addition type process. This estimated concentration is then added to the known spiked concentration for every sample treated, yielding the analyte concentration actually present in the samples. These corrected concentrations are then used in data analysis software (MultiQuant, Mass Hunter) as the actual concentration. This yields an accurate quantification of the analyte, free from interference of the endogenous contribution. This correction has been applied in a production setting on two BHB quantification methods (GC-MS and LC-MS/MS), allowing the rectification of BHB biases of up to 27 µg/mL. The additional error introduced by this correction procedure is minimal, although the exact amount will be highly method-dependent. The endogenous concentration correction process has been automated with an R script. The final procedure is therefore highly efficient, only adding 4 mouse clicks to the data analysis operations.

Development of a Screening Method for Novel Synthetic Opioids Using a DOE Approach and Application to Casework

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In recent years, North America has experienced a considerable growth in mortality related to misuse of prescribed opioids. This “opioids crisis” gained even greater momentum with the apparition of novel synthetic opioids (NSO). These new psychoactive substances (NPS) are derived from prescribed opioids or failed pharmaceuticals, some examples include carfentanil, furanylfentanyl and U-47700. NSO present a high degree of structural similarity and often low biological concentrations, resulting in a clear analytical challenge for forensic toxicology laboratories. The present work describes the development of an LC-MS/MS screening method for 57 NSO using a Design of Experiments (DOE) approach to optimize instrumental conditions (flow rate, column temperature, mobile phase composition, etc.). Biological matrices (cardiac and femoral blood, urine) are extracted by protein precipitation and analysed on an Agilent 1200 HPLC coupled to a Sciex 5500 QTrap operated in positive electrospray ionization mode with multiple reaction monitoring (MRM). Fatal opioids intoxication cases analyzed with this method will be presented, including one where an impressive combination of 15 NSO was detected. Ultimately, this method will allow an assessment of the increasing NSO prevalence in cases handled by the *Laboratoire de sciences judiciaires et de médecine légale* (LSJML).

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

Enhanced Immunopeptidome Identification and Quantitation with High-Field Asymmetric Waveform Ion Mobility (FAIMS) Combined with TMT-Labeling.

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The identification of endogenous peptides presented by major histocompatibility complex class I (MHC I) by LC-MS/MS present significant analytical challenges due to their low abundance and the lower charge state distribution compared to tryptic peptides. To enhance the detection of MHC I peptides, we evaluated the use of TMT labeling on a set of 440 synthetic MHC I peptides. TMT labelling enhanced the formation of multiply-charge peptide ions and resulted in a ~20% gain in identification compared to underivatized peptides. Moreover, TMT peptide labeling provided a higher identification score (Ø77 for TMT-label *vs.* Ø50 for underivatized peptides). Next, we evaluated the analytical benefits of high field asymmetric waveform ion mobility (FAIMS). With 50 million B-LCL cells we identified 4564 MHC I peptides with FAIMS compared to 3755 MHC I peptides without. We extended the application of FAIMS and isobaric peptide labeling to the target analysis of MHC I peptides from only 2 million B-LCL cells. MHC I peptides were derivatized with TMT-126 while increasing amounts of MHCs synthetic peptides were labeled with TMT-128 to TMT-131 to generate a calibration curve. TMT signal amplification obtained using synthetic peptides enabled the more precise quantification with FAIMS compared to regular MS3 method.

Quantitative Method to Analyze the Effect of Acetaminophen on Bile Acids in Rat Plasma by LC-MRM

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UQAM

Bile acids (BA) are derived from the metabolism of cholesterol, playing different roles crucial for liver health. They help with the absorption of lipids and cholesterol. The accumulation of BA is a serious sign of chronic diseases of the liver. The different biological functions of BA, and their implication in pathological processes highlight the importance to understand BA profiles in drug-induced liver injury. Acetaminophen is a drug taken to relieve pain and to decrease fever. It is the main cause of acute liver failure in North America. In severe cases, an overdose of acetaminophen can even cause death. An optimized method was developed to quantify BA by liquid chromatography couple to mass spectrometry. This method was employed to visualize the effects of acetaminophen at different dosing levels on the concentration of 14 different bile acids in rat plasma. A simple step of protein precipitation using MeOH was performed to extract BA. Samples were injected onto a HPLC coupled to a Sciex QTRAP 5500 mass analyzer in MRM mode using both positive and negative ion modes. The high sensitivity and specificity helped detect changes in BA occurring as a result of different doses of acetaminophen.

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

Characterization of Human Mycotoxin Metabolites Using Microsomal Incubations and Mass Spectrometry

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Mycotoxins are common food contaminants produced by filamentous fungi and are ubiquitous worldwide. They have deleterious effects on human and animal health, therefore studying and minimizing mycotoxin contamination is of utmost importance today. The objective of this work was to characterize mycotoxin metabolites that can be generated *in vitro* using microsomal incubations and to build an extensive in-house library of these species, for which standard compounds are often not commercially available. These studies were conducted using pooled human liver microsomes to generate and to characterize phase I and phase II metabolites of the following mycotoxins: ochratoxin A, aflatoxins B1, B2, G1 and G2, zearalenone , 7 α-hydroxy-zearalenol, 7 β-hydroxy-zearalenol, zearalanone, 7 α-hydroxy-zearalanol, 7 β-hydroxy-zearalanol, fumonisins B1, T-2 toxin, HT-2 toxin, deoxynivalenol, nivalenol, 15-acetyldeoxynivalenol, 3-acetyldeoxynivalenol, and fusarenon X. High resolution mass spectrometry instrumentation (LTQ Orbitrap Velos) coupled with liquid chromatography was used for the detection and identification of mycotoxin metabolites. Structural elucidation of metabolites was performed using data dependent acquisition and collision-induced dissociation (CID) fragmentation technique. The final in-house liquid chromatography - mass spectrometry library contains 48 metabolites and will be used in future studies to verify if any of these metabolites are present in human plasma samples.

COMPUTATIONAL CHEMISTRY/CHIMIE NUMÉRIQUE

Molecular Simulation of Metalloid and Group 14 Nitride's Mechanical and Electrical Properties

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The differences between group 14 nitrides (Si_3N_4, Ge_3N_4, Sn_3N_4) and metalloid nitrides (Ti_3N_4, and Zr_3N_4) have been studied with quantum theory simulations. Group 14 nitrides have relatively shorter bond length and a higher degree of charge transfer. The plot of density of states indicates that bonding interaction in metalloid nitrides is between the d orbitals of metal atoms with p orbitals of nitrogen. For group 14 elements, their s, p, and d orbitals all contribute to the bonding. Electronic structure calculations with one shot G_0W_0 and LDA-1/2 corrections implemented in the full potential linearized augmented planewave (LAPW) method, showed good agreement with experimental values. The calculated band gaps for group 14 nitrides are 5.03, 2.66 and 1.74 eV for Si_3N_4, Ge_3N_4, and Sn_3N_4, respectively. They are much larger than metalloid nitrides, which are 1.02 and 1.71 eV for γ-Ti_3N_4 and γ-Zr_3N_4. LDA-1/2 method has proven to be an accurate and efficient method in predicting the band gaps of binary nitride. The results from our comprehensive calculations shed light on the stability and the electronic property differences between the group 14 and metalloid spinel nitrides.

Computational Exploration of Reaction Pathways

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Predicting the outcome of a reaction, its kinetics, and the pathways leading to its products requires detailed knowledge of its energy landscape, that is, the energies of all molecular configurations encountered along the reaction. The exploration of energy landscapes is particularly important for enzyme engineering as it can help determine, for instance, the energetic feasibility of a reaction or the possibility of forming new desirable products. Since large numbers of enzyme mutants are typically considered, it is also imperative to make energy landscape exploration less computationally intensive. In this project, we aim to automate the exploration of energy landscapes. We make use of the activation-relaxation technique (ART) [Machado-Charry et al. 2011, J. Chem. Phys. 135, 034102] and modify it to study complex reactions of the type encountered in enzymes. We demonstrate the concept using the double bond migration of propene. Our ultimate goal is to use ART to study enzymatic reactions using a hybrid quantum mechanics (QM)/molecular mechanics (MM) approach, in which the active site of the enzyme is described using QM while the rest of the macromolecule is described using an MM force field

MethylSight: A Computational Approach to the Elucidation of the Methyllysine Proteome

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Lysine methylation is a post-translational modification of proteins that mediates a myriad of cellular processes including DNA damage repair, cell signaling, and metabolism. Recent research suggests that this vastly understudied modification may be more prevalent than previously thought. Unfortunately, the identification and characterization of lysine methylation sites is technically challenging and resource-intensive. For this reason, the elucidation of the methyllysine proteome has remained elusive. Computational approaches have the potential to facilitate rational experiment design and to guide experiments aiming to identify such sites. Machine learning approaches have shown promise for a variety of applications in biochemistry such as protein-protein interaction prediction or protein function prediction, but have had limited success in predicting lysine methylation sites. Here, we present MethylSight, an alignment-free method for predicting lysine methylation sites in proteins. MethylSight combines the ProtDCal feature extractor with a support vector machine classifier to predict sites with a recall and precision that surpass the current state of the art. The MethylSight web server is freely available, and provides researchers with a streamlined tool to investigate putative lysine methylation sites. Altogether, MethylSight is an invaluable resource for researchers interested in this important post-translational modification.

COMPUTATIONAL CHEMISTRY/CHIMIE NUMÉRIQUE

Prediction of Topological Preferences and Energetic Properties of Metal Azolate Frameworks Using Periodic DFT Calculations

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Metal-organic frameworks (MOFs) are microporous materials of emergent technological importance for gas storage and separation, catalysis, sensing devices and other advanced applications. Computational methods are becoming increasingly important for exploring structure-property relationships in MOF materials, and providing tools for target-specific design of next-generation materials. This presentation will outline our recent advances in using periodic density functional theory (DFT) calculations for characterizing and even predicting MOF structures. We show how periodic DFT calculations can be used to explain the thermodynamic pathways observed in mechanochemically-induced topological transformations of MOFs, demonstrating that such reactions proceed towards thermodynamically most stable structures. Stability of MOF polymorphs at ambient conditions is inevitably affected by the entropic contributions related to atomic motion and disorder. We demonstrate how simulations can be used to explain the occurrence of disorder in MOF structures and estimate the corresponding thermodynamic stabilization effects. Finally, we provide a report of the first *ab initio* screening and evaluation of energetic properties of a previously not synthesized class of MOFs based on the recently isolated pentazolate (**pnz**$^-$) ligand. The energy landscapes for Zn(**pnz**)$_2$ and Cd(**pnz**)$_2$ frameworks were calculated, revealing several previously unreported topologies.

Study of Radical Clock Reactions with High-level Computational Technique

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Traditional methods, including pulse radiolysis, flash photolysis and electron spin resonance (EPR), proved to be limited and costly on determining the reaction rate for many radical-molecule reactions. Moreover, the experimentally measured absolute rate constants possess error due to temperature dependence. For more than 4 decades, radical clock reactions have conferred an alternative way for filling the shortage of the traditional approaches. Radical clock is defined by the unimolecular reaction with known rate, and acting as timing device when involved into competing radical-molecule counterpart. Ring closure, ring open and 1,2-migration are examples of such type reactions. In this project, we aim to use the state-of-art high-level computational techniques for accurately predicting the rate for sets of ring open radical reactions and its reverse reactions. The geometry optimization and frequency will first be performed under CAM-B3LYP/def2-QZVPP and then with correction of dispersion effect from D3BJ. The reaction barrier calculations will be implemented by DLPNO-CCSD(T)/CBS method with aug-cc-pVXZ basis set for accurately including correlation energy.

NANOCHEMISTRY/NANOCHIMIE

Nanogels UCST à Base de Poly(acrylamide-co-acrylonitrile) Réticulés par un Colorant à Base de Nickel Bis(dithiolène) Capable d'Absorber dans le Proche Infrarouge et Évaluation de leur Efficacité Photothermique

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La libération contrôlée de médicaments induite par la lumière proche infrarouge (NIR) constitue actuellement un enjeu majeur dans le domaine de la médecine non-invasive. Les matériaux démontrant un effet photothermique sont particulièrement convoités afin de coupler traitements hyperthermiques et chimiothérapies.

Cette étude reporte la synthèse de nanogels thermo et photosensibles à base de poly(acrylamide-co-acrylonitrile). Ce copolymère possède une thermosensibilité positive (UCST) et son choix a été motivé par la possibilité de contrôler sa température de transition de phase en faisant varier le ratio molaire entre l'acrylamide et l'acrylonitrile. Ces nanogels ont été réticulés par l'intermédiaire d'un complexe à base de nickel bis(dithiolene). Ce composé est capable d'absorber la lumière proche infrarouge et de restituer cette énergie sous forme de chaleur. Ainsi, l'exposition de l'échantillon à une source NIR génère l'élévation de la température au sein des nanoparticules, entraînant la transition de volume positive des nanogels. La dilatation du réseau tridimentionnel permet la libération par diffusion de petites molécules. Le comportement thermosensible des nanogels a été étudié par différentes méthodes lors des deux mécanismes de transfert de chaleur ; par conduction et radiation. De plus, l'efficacité de libération contrôlée d'un modèle de molécule hydrophobe (Nile Red) a été démontrée par fluorescence.

BIOCHEMISTRY/BIOCHIMIE

Non-Histone Substrates for Histone Methyltransferases: Investigating MLL4-Dependant Methylation of 53BP1 and Cfp1

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Histone methylation has long been established as an important transcriptional regulatory mechanism. The methylation reaction is facilitated by a class of enzymes known as histone methyltransferases. Though the name suggests these enzymes are only active on histone substrates, it is becoming apparent that histone methyltransferases interact with many non-histone proteins. Recent evidence suggests that non-histone protein methylation plays a role in many signaling pathways and regulatory mechanisms, but the scope of these interactions is unclear, and the many histone methyltransferases have yet to be probed for additional substrate activity. Utilizing a synthesized in vitro and in silico experimental approach, we suggest that the histone lysine methyltransferase mixed lineage leukemia 4 (MLL4) plays a role in the DNA-damage response (DDR) through the methylation of p53 binding protein 1 (53BP1), and in upstream transcriptional regulation through the methylation of CxxC finger protein 1 (Cfp1). We posit MLL4 methylates 53BP1 within its methyl-binding Tudor domains, potentially modulating 53BP1's ability to bind methylated histone 4 during the DDR. In addition, we propose that MLL4 methylates Cfp1 within its SET interacting domain, blocking Cfp1's association with the histone methyltransferase complexes Setd1A and Setd1B, ultimately disrupting complex formation and subsequent downstream regulatory activity.

BIOCHEMISTRY/BIOCHIMIE

Interaction of Bacterial and Cancer Cells Model Membranes with GL13K: An Antimicrobial Peptide with Anticancer Activity

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GL13K is a thirteen amino acid peptide with broad-spectrum antimicrobial and antibiofilm activity at low MICs, while it is not hemolytic. Thus, this peptide is attractive for therapeutical applications. However, its mechanism of action remains unknown and there are no reports of its anticancer potential. Here, we analyzed the interaction of GL13K with two bacterial model membranes through circular dichroism, PM-IRRAS and X-ray scattering techniques for gaining insight on the structural aspects governing its activity. GL13K displayed a predominantly crystalline b-sheet conformation in presence of bacterial models at different peptide/phospholipid ratios. However, the model membrane with lower surface charge led to greater proportion of unstructured peptide and to slower peptide's insertion in monolayers, suggesting that higher negative charge in periplasmic membranes favors GL13K's interaction. Additionally, D- and L- peptide enantiomers were assessed for anticancer activity in a cancer cell line. D-GL13K showed greater cytotoxicity, supporting that D-enantiomers tolerate the action of proteases *in vitro*. Interestingly, GL13K enantiomers do not undergo conformational changes upon interacting with liposomes mimicking a cancer cell phospholipid membrane. These results provide a better insight into the interaction of short peptide-based antibiotics with bacterial membranes and show the new potential for GL13K application in cancer therapy.

Regulation of SUMOylation, Phosphorylation and Ubiquitination in Response to Arsenic Trioxyde, a Therapeutic Agent Used in the Treatment of Acute Promyelocytic Leukemia

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Acute promyelocytic leukemia (APL) is a cancer of white blood cells characterized by the accumulation of immature granulocytes called promyelocytes. The disease is caused by a chromosomal translocation of the RARα gene which, in the majority of cases, occurs reciprocally with the PML gene, leading to the expression of the PML/RARα fusion protein. One of the therapeutic agents used to treat this leukemia is arsenic trioxide. Despite the fact that its effectiveness in treating the disease is proven, the molecular mechanisms through which the agent passes are not fully characterized. The mechanism may involve SUMOylation and it is known that the PML protein is SUMOylated in response to treatment with arsenic trioxide. This introduces the idea that other integral proteins may exhibit changes in their post-translational modification profiles, such as SUMOylation, ubiquitination or phosphorylation. Quantitative proteomic analysis identified 226 proteins significantly regulated by SUMOylation in HEK293 cells treated with arsenic trioxide, some of which are known to be involved in cell cycle arrest, senescence and apoptosis. A better understanding of the mechanism may provide further insights on improving the efficiency of arsenic trioxide as a treatment for APL, as well as expanding its applicability in the treatment of other cancers.

BIOCHEMISTRY/BIOCHIMIE

Using Solid-State NMR to Fully Assign Starch Chemical Shifts: Purified and In-Cell Carbohydrate Polymer Characterization

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Starch is the most abundant energy storage molecule in plants and is, with cellulose, the most abundant polysaccharide in nature. This glucose polymer consists of alternating amorphous and crystalline domains which can be found into two different structures, i.e., A and B-types with specific physicochemical properties and valued differently in the food industry, for example. Using two-dimensional (2D) high resolution solid-state NMR on ^{13}C labelled starch obtained from *C. reinhardtii* microalgae, we established complete and unambiguous assignments for starch and its constituents (amylopectin and amylose) in the two crystalline forms and in the amorphous state. The 2D-INADEQUATE experiments under magic-angle spinning (MAS) offer high resolution and spectral dispersion enabling assignment of hereto unreported non-reducing end groups. This work illustrates how the INADEQUATE experiment can be used to garner information on organic disordered solids. Furthermore, we show how these NMR methods enable the detection and identification of starch *in situ* in intact cells, as well as by-products, therefore eliminating time consuming and potentially altering purification steps. We thus provide a solid basis for the NMR study of starch structure, its chemical modifications or biosynthesis in living microorganisms, making *in situ* NMR a powerful tool to study molecules directly in the cell.

The Investigation of the Chemical Ecology of Geosmin

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Some autotrophs, heterotrophs, prokaryotes and eukaryotes all produce a natural product ubiquitously: “Geosmin”. It is a volatile organic compound (VOC) responsible for the smell of rain that we can detect at 5ppt. This sesquiterpene is produced during the mevalonate or the MEP pathway depending on the producer. However, even though geosmin is produced everywhere, the understanding of its chemical ecology is yet to be discovered. This natural product can potentially attract or repel other organisms, it might also permit interspecific communication. We are working to understand this fascinating chemical and the effect it has on the survival of the bacterial predator *Myxococcus xanthus*.

Environmentally Benign Reactions on Biomass-Derived Furans as a New Strategy for the Synthesis of Complex Value-Added Materials

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Concordia University

High demand and uncontrolled use of petroleum feedstocks has had a tremendous negative impact on the environment. Nowadays, much attention is being paid to biomass as a source of organic starting materials, and the U.S. department of Energy has highlighted furans derived from hemicellulose as potential building blocks for chemical synthesis, such as 5-hydroxymethyl furfural (HMF) and 2,5-furandicarboxylic acid (FDCA).

The synthesis of high-value biomass derived 2,5-diaryl furans has been achieved successfully from good to excellent yields with a wide scope of coupling partners of aryl halides and FDCA, and the article has been published already with the results and protocols developed. Keeping in mind that FDCA comes from direct oxidation of HMF, a route to access 2,5-assymetric furans was achieved. Selective oxidation of the aldehyde moiety has not been reported under mild accessible conditions, therefore a solvent-free mechanochemical assisted selective oxidation was studied to synthesize the 5-hydroxymethyl-2-furoic acid. Decarboxylative cross-coupling and oxidation of the alcohol gave yield to the new substrate for the decarboxylative cross-coupling, therefore, achieving the convenient synthesis of 2,5-diaryl non-symmetric furans. Additionally, initial results on the decarboxylative cross-coupling polymerization of FDCA and aryl dihalides are presented a new green and sustainable strategy to obtain furan-aryl co-polymers.

Sequential Palladium-Catalyzed Decarboxylative Cross-Couplings for the Facile Synthesis of Non-Symmetic Arylated Thiophene

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Concordia University

Currently, classical Pd-catalysis is used for the preparation of organic diodes and organic photovoltaics. Some issues with this class of reaction, however, are the need for organometallic reagents and the difficulty in carrying reactive groups into a synthesis. In recent years, decarboxylative cross-coupling (DCC) has emerged as versatile methodology for carbon-carbon bond formation, offering an alternative that drastically reduces the production of organometallic waste, as the protocol utilizes the electronics of the heterocycle to preclude the need for a bi-metallic catalytic system. DCC can be applied to the functionalization of thiophene, a heteroaromatic that has become a dominating motif in burgeoning opto-electronic industries. This allows for a desirable access to non-symmetrical thiophenes, as non-symmetry greatly increases the library of possible structures. For this aim, the Forigone-Bilodeau procedure has been adapted for tolerance of an adjacent ester moiety, which can then be quickly saponified to an acid for access to a variety tri-aryl motives via tandem coupling reactions. Conditions for the reactions were optimized for waste reduction by increasing the atom economy of the reaction, and also minimizing the amount of purification steps and the subsequent production of solvent waste.

Synthesis of Tunable Anion Receptors using Palladium-Catalyzed Decarboxylative Cross-Coupling Reactions

C. Buonomano

Concordia University

Anions are ubiquitous in the natural world and are critical in the circle of life. The misregulation of anions' function can have serious consequences (e.g. osteoporosis, cystic fibrosis). Anion receptors will act as a surrogate when endogenous receptors or proteins are dysfunctional. Anion receptors designed for a specific anion and tuned for an increased binding strength and lipophilicity, they have been shown to restore transmembrane transports of anions and may find use in medicinal chemistry. The synthesis of tunable anion receptors can be achieved via palladium-catalyzed cross-coupling reactions. Classical methods have the drawback to produce stoichiometric amounts of organometallic reagents byproducts. Recently, decarboxylative cross-couplings have emerged as advantageous alternative to classical methods. In order to further increase the attractiveness of our method and extend its versatility, it is crucial to find some synthetic applications involving them to synthesise new biologically active molecules. The purpose of this research project is to apply the C-C bond formation methodology developed by our group, and use it for the synthesis of various tunable anion receptors.

Utilizing Decarboxylative Cross-Coupling for a Discrete Library of Oligothiophene

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In recent years, oligothiophene have become promising materials for green energy applications, such as plastic solar cells. Traditionally, conjugated heteroarenes are synthesized by Kumada, Stille, and Negishi cross-coupling reactions. The major drawback of these reactions is the stoichiometric amount of organometallic by-product. Our group utilizes carboxylic acids and salts as nucleophilic cross-coupling partner, which provides regioselectivity and good to excellent yields with a broad range of substrates. These strategies have been proposed as milder and environmental benign alternatives to traditional cross-coupling reactions, as gaseous by-products are extruded from the reaction. This research will be exploring the possibility of utilizing decarboxylative cross-coupling reaction to prepare a discrete library of oliothiophene. Numerals symmetric oligothiophene have been synthesized with good to moderate yield.

Catalytic *N*-Modification of a-Amino Acids and Small Peptides with Phenol under Bio-Compatible Conditions

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Amino acids are bio-renewable, *C*-chiral, nitrogen sources with important applications in chemistry and biology. Our laboratory has developed novel methodologies through which these building blocks can be arylated or cyclohexylated by using 2-cyclohexen-1-one or phenol, respectively. By using a phenolic compound as the *N*-alkylating reagent we can circumvent the need of alkyl halides and protecting groups, while generating water as the sole by-product. In addition, phenol represents a sustainable alternative to current alkylating reagents due to its wide availability as the main constituent of lignin. Upon optimization we found that *N* -arylation is achieved using 2-cyclohexen-1-one as the coupling partner with up to 74% yield; while phenol is successfully used to *N*-cyclohexylate 17 out of the 20 natural a-amino acids as well as small peptides in excellent yields in water at room temperature.

Burkholderia Pseudomallei and *Burkholderia Mallei* Synthetic Lipopolysaccharide Mimics as Potential Vaccine Candidates

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Gram-negative bacteria (GNB) *Burkholderia pseudomallei* (*Bp*) and *Burkholderia mallei* (*Bm*), endemic in tropical and subtropical regions, are respectively the causative agents of melioidosis and glanders. Due to the threat they represent for the society, these GNB have been classified as potential bioterrorism weapons by the *Centers for Disease Control and Prevention*.

At their cell surface, GNB possess different polysaccharides, including lipopolysaccharides (LPS). The O-antigen (OAg) portion constitutes the virulence determinant and protective antigen of *Bp* and *Bm*, and consists in a repetition of a disaccharide unit composed of glucose and 6-deoxy-talose moieties, the latter being diversely methylated and acetylated. The antigenic and immunogenic potential of oligosaccharides mimicking the main intrachain and terminal epitopes have already been reported by our team. In this context, a synthesis pathway enabling the preparation of tetrasaccharides akin to *Bp* and *Bm* LPS through a [1 + 1 + 1 + 1] glycosylation methodology based on the use of orthogonal and participating protecting groups was developed. Selective reactions were conducted and anomerically pure oligosaccharides were isolated, highlighting the suitability of the developed method for the synthesis of complex oligosaccharides. The tetrasaccharides under study could find usefulness in the development of prophylactic measures against melioidosis and glanders.

Computational Design and Synthesis of Asymmetric Catalysts

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Asymmetric catalysts are an important and integral component in the synthesis of chiral compounds. However, the discovery process of asymmetric catalysts is slow, tedious and cost-inefficient. Our group has developed a novel computational tool, Ace (Asymmetric Catalyst Evaluation), designed to predict the stereochemical outcome of reactions using newly designed catalysts. Ace does not require expertise in computational chemistry and is meant to be used by organic chemists to evaluate the selectivity of newly designed catalysts **prior** to synthesis. As such, the catalyst structure can be optimized *in silico* and only a small number of catalysts would need to be synthesized and tested. Ace is part of the Virtual Chemist platform that can be used to create a library of potential catalysts and test them *in silico* for their selectivity, prior to synthesis. Current efforts in our lab involve the computational-aided design, synthesis and testing of novel organocatalysts, with a focus on the Diels-Alder cycloaddition. We will present the development of the software and its application to the discovery of novel Diels-Alder cycloaddition catalysts. This has been done by virtual-screening conducted on a database (virtual-library) of previously reported asymmetric compounds. In addition, the future potential of the software will be presented.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Heavy Metal Sensitivities of Gene Deletion Strains for *ITT1* and *RPS1A* Connect their Activities to the Expression of *URE2*, a Key Gene Involved in Metal Detoxification in Yeast

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Heavy metal and metalloid contaminations are among the most concerning types of pollutant in the environment. Consequently, it is important to investigate the molecular mechanisms of cellular responses and detoxification pathways for these compounds in living organisms. To date, a number of genes have been linked to the detoxification process. The expression of these genes can be controlled at both transcriptional and translational levels. In baker's yeast, *Saccharomyces cerevisiae*, resistance to a wide range of toxic metals is regulated by glutathione S-transferases. Yeast *URE2* encodes for a protein that has glutathione peroxidase activity and is homologous to mammalian glutathione S-transferases. The *URE2* expression is critical to cell survival under heavy metal stress. Here, we report on the finding of two genes, *ITT1*, an inhibitor of translation termination, and *RPS1A*, a small ribosomal protein, that when deleted yeast cells exhibit similar metal sensitivity phenotypes to gene deletion strain for *URE2*. Neither of these genes were previously linked to metal toxicity. Our gene expression analysis illustrates that these two genes affect *URE2* mRNA expression at the level of translation.

Molecular Control of Genome Architecture

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BACKGROUND: The nuclear lamina regulates genome organization. Lamin A and Lamin B receptor are key proteins required for heterochromatin tethering. Adult mouse rod photoreceptors express neither of these proteins, resulting in a unique nuclear architecture which makes them a convenient model for studying molecular determinants of genome organization.

OBJECTIVE: We propose to use mouse rod photoreceptors as an assay system for tethering sufficiency. We hypothesize that the C-terminus of Lamin A binds heterochromatin. Our goals are to identify the critical domain responsible for heterochromatin tethering, and to elucidate the genomic and transcriptomic consequences behind it.

METHODS: To determine how tethering proteins affect genome organization, we ectopically express them in mouse rods. We inject the plasmid DNA into the eye and transfect it by in vivo electroporation. ATAC-seq and RNA-seq will help to determine the genomic and transcriptomic changes of the observed phenotype changes of Lamin A.

RESULTS: Lamin A causes reorganization of the rod nucleus and is sufficient for heterochromatin tethering. GFP-tagged Lamin A doesn't affect the genome.

CONCLUSIONS: The Lamin A C-terminus might be the key for heterochromatin tethering. N-terminal occlusion also appears to be function-blocking, suggesting that there are multiple domains containing affinities for different types of heterochromatin.

The Role of NPHP5 in Basal Feet Formation

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Cilia are microtubule-based structures found at the surface of almost all eukaryotic cells. Although cilia are vital organelles both physiologically and clinically, the process of ciliogenesis is poorly understood. We have found that a previously characterized protein, NPHP5 localizes to the distal part of centrioles and is required for ciliogenesis. We hypothesize that characterizing the precise localization of NPHP5 would allow for a better understanding of how NPHP5 is involved in ciliogenesis. There are structures associated with the distal part of basal bodies, transition fibers (TFs) and basal feet (BF). TFs and BF are tiny protrusions equivalent to distal appendages (DAs) and subdistal appendages (SDAs) of mother centrioles. We did 3D-SIM to assess the localization of NPHP5 and observed that NPHP5 co-localizes with two known SDAs/BF proteins, ninein and Cep170. In the absence of NPHP5, some of the BF proteins were mis-localized, revealing a requirement of NPHP5 for organizing BF. In contrast, depletion of NPHP5 had no effect on SDAs. We also determined the close association of NPHP5 with BF protein ninein by proximity igation assay. Thus, in addition of its previously known role in ciliogenesis, NPHP5 regulates BF structure and assembly.

Synthesis of 2-thiouracil PNA Monomer for Fmoc-Based Synthesis of Pseudo-Complementary Oligomers

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Pseudo-complementary nucleobases are modified nucleobases which exhibit normal base pairing with unmodified complementary nucleobases; however, will not undergo base pairing with other pseudo-complementary nucleobases. 2,6-Diaminopurine, an adenine analogue, and 2-thiouracil (2-thiothymine) are two pseudo-complementary nucleobases which undergo normal Watson-Crick base pairing with thymine and adenine respectively; however, steric hindrance prevents diaminopurine:thiouracil(thiothymine) base pairing. Until recently, pcPNAs were synthesized via Boc-based oligomerization chemistry which is currently less popular than the Fmoc-based strategy[1].

This research describes the development of a Fmoc protected thiouracil PNA monomer with an acid labile protecting group for use in standard SPPS[2]. Our studies revealed that the 2-methoxybenzyl protection is unexpectedly an acid resistant group, while the acidolysis of the 4-methoxybenzyl protecting group suggests the protecting group is removed under standard boc-based oligomerization conditions[3]. Thus, the thiol protection is likely unnecessary for oligomerization. To test this hypothesis, oligomerization was performed using an unprotected thiouracil PNA monomer and compared to previous oligomerization conditions. The synthesis uses an orthogonal protection strategy where the nucleobase is deprotected under standard acidic deprotection and resin cleavage conditions, while oligomerization occurs under basic conditions.

Genes of the Undead: Do Hibernators and Zombies Display Similar Expression Profiles?

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Tight genetic and epigenetic regulation is required to sustain the complex homeostasis that is life, and it seems that a degree of this regulation continues into death. Post-mortem transcriptome studies have identified a subset of genes that appear to come alive hours and days after organismal death. These so-called 'zombie genes' have been functionally characterized into various stress-responsive processes. In this study, we hypothesized that hibernation, representing the closest living and natural mammalian phenomenon to death, would display similar gene expression profiles to the undead genes that are activated after death. Yet despite the profound metabolic rate depression and severe slowdown of most biological and physiological functions experienced during hibernation, our multi-tissue (liver, heart, brain cortex, hypothalamus, brown adipose, skeletal muscle, bone marrow) expression analysis of 45 representative 'zombie genes' in hibernating ground squirrels (*Ictidomys tridecemlineatus*) showed little in common with the pattern of gene upregulation observed after organismal death. This showcases the extent to which hibernators shut down gene transcription, surviving only on the transcripts and proteins that are necessary and required for survival, and do not require the expression of a set of zombie genes that could correspond to the cell's last resort in extremely stressful environments.

Resensitization of *Salmonella Enterica* Ser. Typhimurium to the Macrophage Metabolite Itaconate *In Vitro* and *In Cellulo*

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Itaconate is a metabolite produced in macrophages that has an important role in the immune response and a vital role in managing bacterial invasion. This metabolite is an effective inhibitor of isocitrate lyase, an essential enzyme for intracellular pathogenesis. Some pathogens such as *Salmonella* Typhimurium have evolved to degrade itaconate, thus allowing it to survive inside macrophages. We have discovered a compound that inhibits the degradation of itaconate by *S.* Typhimurium which consequently gives these bacteria the phenotype of bacteria which lack the itaconate degradation pathway. We developed a checkerboard assay to verify the sensitivity of bacteria to itaconate in the presence or absence of itaconate degradation inhibitors. This was instrumental to demonstrate the synergistic effect of itaconate degradation inhibitors with itaconate for killing *S.* Typhimurium. Using *S. typhimurium* infected BV2 cells incubated in itaconate, we have also shown that the compound helps to clear the infection.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Role of Oxygen on Nuclear Factor Erythroid-2-like 1 (NFE2L1) Function and Stability

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Oxidative stress has been recognized as one of the key players involved in human aging and progression of many chronic diseases, including cancer. Cells undergo oxidative stress when the overproduction of reactive oxygen species within the cell outweighs its antioxidant defenses. As a defence mechanism, a series cytoprotective genes are initiated and regulated by various transcription factors in order to minimize oxidative damage to the cell. Nuclear factor erythroid-2-like 1 (NFE2L1) is a transcription factor found to be one of the vital regulators of antioxidant and detoxification genes. However, as a primarily endoplasmic reticulum (ER) membrane bound transcription factor, the mechanism of how NFE2L1 is being processed, translocated from ER to nucleus, post-translational modified and degraded are still unclear. This study aimed to determine whether NFE2L1 is regulated, in an oxygen-dependent manner, by hydroxylation. A potential hydroxylation site was identified on NFE2L1 that may be target for modification by Prolyl Hydroxylase 2 (PHD2). Oxygen-dependent hydroxylation of NFE2L1 may affect its function under hypoxic (1% O2) conditions when hydroxylation is absent. Enhancement of NFE2L1 function under hypoxic conditions will be further investigated as a potential target for therapeutic peptides that will reduce its hydroxylation and augment its antioxidant and detoxification activities.

BIOCHEMISTRY/BIOCHIMIE

Maturation of Heme Proteins in *Saccharomyces cerevisiae*

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Heme is an essential prosthetic group in key proteins involved in cell respiration, antioxidant defense and xenobiotic detoxification. Heme biosynthesis is finalized by Fe^{2+} insertion into protoporphyrin IX by ferrochelatase (FECH) in mitochondria. However, it is not known what proteins receive heme from FECH. Since heme from cytochrome c peroxidase (Ccp1) is recruited for the maturation of peroxisomal/mitochondrial apocatalase (apoCta1), we hypothesized that Ccp1 may receive heme from FECH. As a starting point, we analyzed GST-apoCcp1 pulldowns from the mitochondrial enriched fraction (P10) of 1-day yeast cells. To optimize the pull down of membrane-associated proteins, we added detergents to the P10 fraction. Since enzyme activities (cytochrome c oxidase and Ccp1) were highest in P10 with N-octylglucoside (NOG), we performed the GST-apoCcp1 pulldowns with 0.6% NOG present. LC-MS/MS analysis detected 64 protein interactions of apoCcp1 but not FECH so we increased the GST-apoCcp1:P10 (i.e., bait:prey) ratio from 1:1 to 1:5 and detected 363 apoCcp1 interactors, including FECH and Pet9. Hence, heme may be delivered from FECH to apoCcp1 via Pet9, a known heme binding transmembrane protein. Other interactors that we identified suggest that Ccp1 links heme trafficking and antioxidant defense in yeast cells.

BIOCHEMISTRY/BIOCHIMIE

Visualizing the Heme Status of a Protein Using Green Fluorescent Protein

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Apocatalase A (Cat1) maturation involves recruitment of heme from cytochrome c peroxidase (Ccp1) in yeast mitochondria. Thus, tracking Ccp1's heme status in live cells is of interest but has not been reported to date. Heme is a highly efficient quencher of green ApoCcp1-GFP exhibits a fluorescence lifetime of 2.86 ns whereas holoCcp1-GFP decays with two lifetimes, 0.96 ns and 2.45 ns. The fractional amplitude of the 0.96-ns lifetime increases linearly with heme loading of apoCcp1-GFP. With this knowledge, we examined by fluorescence lifetime imaging microscopy (FLIM) the heme status of Ccp1 in the live yeast expressing Ccp1-GFP. From GFP lifetime amplitudes, we find that Ccp1-GFP is ~90% heme loaded and resides in the mitochondria of 2-day cells. In contrast, in 7-day cells, half of Ccp1-GFP is extra-mitochondrial and 100% heme-free. Overall, our unprecedented study reveals the power of FLIM in monitoring both the heme status and location of a GFP-fusion protein in live cells

Development of Enzyme Activity Assay to Study Substrate Selection KDM5/JARID1 Family of Lysine-Specific Histone Demethylases

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The KDM5/JARID1 family are α-ketoglutarate and Fe(II)-dependent lysine-specific histone demethylases that are characterized by their DNA-binding ARID domain and Jumonji catalytic domains. This family of enzyme have been well-established to facilitate the removal of tri- and dimethyl modifications from lysine 4 of histone H3 (i.e., H3K4me2/3). The KDM5-facility demethylation of this residue enables accessibility of local genes for active transcription. Although H3K4me2/3 is the only currently known substrate, the KDM5 family has been shown to have a direct impact on tumorigenesis; although it is unclear how much of KDM5's tumerigenic activity is attributable to H3K4me2/3 demethylation alone, and a number of yet to be discovered oncogenic KDM5-substrates that likely exist. By creating a library of 160 mutated peptide substrates whose sequences are systematically altered from the H3K4 sequence, relative KDM5 substrate preference can be determined and used to identify potential unknown substrates. My research to date has identified numerous potential non-histone protein substrates for KDM5A *in vitro*. Many of the identified methylated protein substrates identified are involved in significant cellular processes or signaling pathways, such as growth signaling (VEGFR1 and KRas) and DNA damage response (p53). Of these protein substrates, KDM5A displayed significant activity towards p53 K370me3 substrate *in vitro*.

A Chimeric Nucleobase - Phenylazo Derivative as an Intrinsic Nucleobase Quencher

G. Park*, R. Hudson

Western University

Molecular beacons are important bioanalytical probes, most often constructed from a single-stranded oligonucleotide, which has been labeled at opposite termini with a fluorophore and a quencher. When the fluorophore and quencher are in close proximity, ideally, no fluorescence is observed due to Fluorescence Resonance Energy Transfer (FRET). DABCYL (4-dimethylaminoazobenzene-4'-carboxylic acid) is commonly used as a quencher in molecular beacons; however, DABCYL is unable to form a base-pair and is conventionally placed as an overhanging residue. This produces a DABCYL moiety wherein the chromophore has substantial mobility and limits the types of other conjugates that can be prepared. In order to overcome these limitations, we have embarked on the synthesis of peptide nucleic acid (PNA) analogues possessing DMPAU (5-[(4-dimethylaminophenyl)diazenyl]uracil) and NPhpC (6-(4-nitrophenyl)pyrrolocytosine) nucleobases which have the ability to quench fluorescent emission in a molecular beacon construct, while forming complementary base pairs by canonical hydrogen bonding. This allows insertion of the nucleobase quenchers next to the fluorescent nucleobase in stem sequence of the molecular beacon. DMPAU and NPhpC PNA analogs provide reasonable quenching effects toward blue fluorophores. The hydrogen bonding study with ^{1}H NMR titration shows DMPAU has a similar hydrogen bonding energy (Ka) for adenine, as the A-T base pair.

Carbazole-Based Complexes as Catalysts

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Unlike coal and oil-based fuels, the combustion of hydrogen only produces a 'green' byproduct - water - and energy. But H_2 does not occur naturally, so it is only a truly 'green' fuel (carbon-neutral) if it can be made without producing CO_2. Currently it is produced by steam methane reforming (SMR, generates CO_2), biomass gasification, and fermentation, and electrolysis of water ('green' if the electricity is generated by renewables). Catalysts to lower the energy required to generate H_2 are being sought: molecular cobalt catalysts are being targeted, not least as Co is abundant, low cost and toxicity. We have tested 17 mono- to di- and tetra-nuclear cobalt complexes for photocatalytic hydrogen evolution: all were found to be active. A diphenylamine-based macrocyclic cobalt complex (right) was the most active. Hence my aim is to design, prepare and test some carbazole-based analogues of this macrocycle, aiming for improved catalysts - more efficient and more stable in solution during catalysis. Acknowledgements: Thanks to the University of Otago (PhD scholarship) and Catalyst Seed Fund (Ministry for Business and Innovation, NZ), for travel support.

High Photocatalytic Efficiency of Molecular Ru-Co System for Solar Fuel Generation

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UdeM

Nature has been using sunlight as its main energy source to oxidize water and fix CO_2 to produce carbohydrates for over a billion years. Molecular artificial photosynthesis aims to mimic nature by extracting electrons from water and reducing protons or others organic compounds (CO_2...) in order to store solar energy in chemical bonds. Since the combustion product of hydrogen is water, this chemical conversion acts as a promising solution for renewable energy. Nowadays, the pure inorganic materials show still limitations or costly reaction conditions. Tuning the properties of molecular photocatalytic center by the design of metal-ligand interaction shows infinite possibilities of creation. Here, we highlight the efficient photocatalytic activity of a mononuclear Ru-Co couple system for hydrogen generation. Amide polypyridine based Ru in association with derivative oxime based Co catalysts are investigated under various wavelength of irradiation and their photo-catalytic activity is discussed.

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

Overcoming the Barriers to Characterizing Strongly Absorbing Aerosol Particles

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Absorbing aerosol particles are of interest in climate science since they absorb and reemit radiation from the sun leading to atmospheric warming. Single particle studies are of great importance as they remove the effects of ensemble averaging and allow for precise determination of particle size and composition. The successes seen in the optical trapping and characterization of single weakly absorbing aerosol particles have proven to be difficult to extend to strongly absorbing particles. Here we present an optical set-up capable of trapping single absorbing particles. We collect white light scattering spectra of trapped dye-doped polystyrene beads. We show that the real and imaginary parts of the refractive index of a particle can be determined through the use of a Lorentzian oscillator model, the Kramers-Kronig relations, and broadband light scattering measurements. The size of a single particle can be simultaneously be found by maximizing the correlation between a collected spectrum and a library of simulated spectra.

Detection of Nanoscale Phase Separation in Nanoparticles with Mixed Ligand Shells by Solid State NMR

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“Patchy particles” where the surface is anisotropically patterned through variation in the surface composition, can form different colloidal crystal structures and have applications as interface stabilizers, in catalysis and targeted drug delivery. “Patchy nanoparticles” can be formed by adsorbing two chemically different polymer chains that will spontaneously phase separate. Although there is growing interest in polymer based patchy nanoparticles, the majority of the studies have been theoretical rather than experimental due to difficulties in preparing significant quantities of nanoparticles with controlled polymer ratios, while experimental validation has also lagged due to the lack of appropriate tools to detect nanoscale phase separation.

As a model system, metal oxide NPs with polystyrene and poly(ethylene oxide) ligands with different ratios were prepared through a simple exchange process. Solution and solid-state NMR experiments designed to characterize the phase separation on different length scales were applied to characterize the nanoparticles with mixed polymer ligands and their assemblies in response to different solvent mixtures was explored.

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

Unraveling the Microstructure of Molecularly Doped P3HT by Thermally-Induced De-Doping

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Molecular doping of organic semiconductors (OSCs) demands control over more parameters than just energetic matching of donor and acceptor. Knowledge of beneficial packing structures of the OSC with the dopant may facilitate improvement in processing methods and molecular design rules. In a novel approach, we investigated the complex microstructure of poly(3-hexylthiophene) (P3HT) p-doped with the strong electron acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ). We exploited temperature-induced dopant desorption as a tool for tuning the doping concentration as a quasi-singular parameter. Through scattering (GIXRD) and spectroscopic techniques (FTIR, UV/vis/NIR), we find p-doped P3HT to comprise regions where a) the backbone packs with the dopant anions in a metastable, co-crystalline structure and b) where the pristine polymer backbones pack closely. Additionally, ionized F4TCNQ can be found dispersed in the alkyl chain region of P3HT. It is revealed that the dopants within the mixed crystalline phase are the thermally least stable ones. Notably, they appear to play no crucial role for charge transport since the thin film conductivity remains unaffected as this phase recedes. Overall, our findings demonstrate the potential value of thermal de-doping in accessing structural information otherwise occluded by the intrinsic structural and energetic complexity of doped organic semiconductors.

Aerosol Diffusivity Studies: Single-Particle Experiments Using Optical Traps

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McGill University

Aerosol particles are abundant in the atmosphere and have many impacts on the environment, climate and human health. Whilst they are ubiquitous, aerosols remain one of the least understood components of the atmosphere. One area which requires more research is how aerosols uptake and release water upon changes in the surrounding relative humidity (RH). An aerosol regularly varies in size as a function of RH and until recently, it was thought that aerosols were in equilibrium with the surrounding atmosphere at all times. However, it has been shown that aerosols' size response can 'lag' behind the change in RH, depending on their constituents, by impeding the diffusion of volatile species through the droplet. Secondary organic material (SOM) can represent greater than 50% of an aerosol's mass and are the primary contributors to this effect. Using a highly focussed laser beam, single aerosol particles can be trapped and confined in a cell and studied using light scattering measurements. By varying the RH inside the cell and studying the subsequent response of a trapped aerosol, binary diffusion inside a droplet can be studied along with the mechanism by which SOM can affect this process.

ANALYTICAL CHEMISTRY/CHIMIE ANALYTIQUE

Detection of Crude Oil Contamination using n-Alkane and PAH Diagnostic Ratios

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Frequent consumption of petroleum and crude oil for energy purposes has resulted in the contamination of many natural systems and waterways. However, determining the presence and level of contamination has been difficult due to the complexity of the molecular fingerprint of petroleum and crude oils. Naturally-occurring straight-chain n-alkanes and polycyclic aromatic hydrocarbons (PAHs) in sediments are both commonly used when examining diagnostic ratios for source determination purposes, and these ratios may be affected by the presence of petroleum and crude oil. As such, the diagnostic ratios offer a potential avenue for determining whether crude oil contaminants are present in natural systems. The purpose of this experiment was to determine whether diagnostic ratios of n-alkanes and of PAHs could be used to detect crude oil or petroleum contamination, and at what level of contamination the difference becomes significant. This was accomplished by separating the natural and crude oil hydrocarbons by column chromatography, spiking natural sediment hydrocarbons with crude oil hydrocarbons at different levels, and analyzing the samples by gas chromatography-mass spectrometry (GC-MS).

Identification of Acetaminophen-Related Covalent Protein Binding to Glutathione *S*-Transferase by LC-MS/MS

T. Geib*, L. Sleno

UQAM

Hepatotoxicity of over-the-counter medications, such as acetaminophen (APAP), is resulting in major drug-induced adverse effects. APAP is known to form reactive metabolites, and covalently bind to cysteine residues of hepatic proteins. We have investigated the protein binding of APAP to different glutathione *S*-transferase (GST) isoforms by liquid chromatography-tandem mass spectrometry (LC-MS/MS).

In vitro activation of APAP to *N*-acetyl *p*-benzoquinone imine (NAPQI) was performed with rat liver microsomes or human CYP3A4 Supersomes, while adding recombinant GSTs. Further sample preparation employed tryptic or peptic digestion, coupled to LC-MS/MS analysis. Results between solid-phase extraction and offline LC fractionation have been compared. We have developed two LC-MS/MS based strategies and compared them for target identification.

The first screening technique used a traditional bottom-up proteomics workflow using data-dependent acquisition (DDA) with database searching, with custom modifications for APAP. Then, a targeted multiple reaction monitoring (MRM) method for all cysteine-containing peptides of the individual GST isoforms was optimized. Several cysteine sites were detected as modified in the tested GSTs. Comparison of the performance of DDA and MRM analyses showed that MRM represents a complementary technique to untargeted DDA, with increased site identification and higher throughput.

Studying the Metabolism of Sunscreen Compounds *In Vitro* Using LC-MS/MS

A. Guesmi*, L. Ohlund, L. Sleno

UQAM

The exposure to UV radiation can induce adverse effects on human health, such as immunosuppression and cancers. Sunscreens are used as UV protection agents. However, some UV filters can also act as endocrine disruptors and carcinogens. The metabolism of active ingredients contained in sunscreens was studied using human and rat liver microsomes with LC-HRMS/MS. A focus of this study was to determine if these compounds can form reactive metabolites with potential toxic effects. Six sunscreen compounds, including avobenzone, oxybenzone, homosalate, octisalate, octinoxate and octocrylene, were incubated with human and rat liver microsomes, NADPH and GSH. Controls were prepared without cofactors. Metabolite analysis was performed on a Shimadzu Nexera HPLC coupled with a Sciex 5600 TripleTOF system, in positive and negative electrospray mode. LC separation used a biphenyl reversed-phase column and gradient elution with water and ACN (both with 0.1% formic acid). Data were examined using Metabolite Pilot, and Masterview softwares (Sciex) to find metabolites and adducts formed in these incubations.

We have detected GSH adducts for many of these compounds tested in both human and rat. We also detected hydrolysis products for compounds containing ester groups. High resolution MS/MS data was used for structural elucidation of metabolites and GSH adducts.

Stable-Carbon Isotope Analysis of Carbon Redox End-Members Within Hypoxic Estuarine Sediments

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Concordia University, GEOTOP

Methane (CH_4) and carbon dioxide (CO_2) are redox end-members of organic matter (OM) diagenesis in sediments and are interconverted via bacterial mechanisms (methanogenesis: CO_2 to CH_4; methanotrophy: CH_4 to CO_2). Eutrophication within the St. Lawrence Estuary (SLE) has resulted in hypoxia (low dissolved oxygen levels) in the bottom waters, potentially affecting carbon cycling between CH_4 and CO_2 within these sediments. Stable-carbon isotope analyses of $CH_4$and CO_2 (measured as total dissolved inorganic carbon) provide insight to conversion mechanisms, as well as potential alternative sources or production pathways of these species. These findings can be linked with analyses of other sediment redox species and dissolved organic carbon to model OM diagenesis in hypoxic sediments. Stable-carbon isotope signatures and concentrations of CO_2 transecting the SLE and into the St. Lawrence Gulf will be presented, as well as strategies to link this data with stable-carbon isotope signatures of CH_4.

Determining Isocyanate Exposure in Human Urine by LC-MRM

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Accurate and chronic effects may result from 4,4'-methylene diphenyl diisocyanate (MDI), 2,4'-toluene diisocyanate (2,4-TDI), 2,6'-toluene diisocyanate (2,6-TDI) and 1,6'-hexametylene diisocyanate (HDI) exposure, with the primary manifestation being occupational asthma. After absorption in the body, these molecules get metabolized through acetylation or conjugation reactions before their elimination into urine.

The hydrolysis of urine samples releases the corresponding free amines as biomarkers of exposure: 4,4'-methylenedianiline (MDA), toluenediamine (2,4-TDA and 2,6-TDA) and hexamethylenediamine (HDA). In this study, we have developed and optimized a LC-MRM method to measure isocyanate exposure. Urine samples were acidified and heated to form free MDA, TDA and HDA, followed by a neutralization step and liquid-liquid extraction. The extracts were derivatized with acetic anhydride and separated on a reverse phase HSS T3 column coupled to a triple quadrupole platform in positive MRM mode. Chromatographic separation was optimized to ensure retention and minimize matrix effects for the four analytes. The method was developed considering the biological guidance value (BGV) of MDI at 50 nM, the biological index of exposures (IBE) of TDI (2,4-TDI and 2,6-TDI) and HDI at 5 µg/g and 15 mg/g creatinine, respectively.

In Vitro Oxidative Metabolism and GSH Adduct Formation of Bisphenol A Analogs by LC-MS/MS

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UQAM

Bisphenol A (BPA) is widely used in the production of polycarbonate plastics and epoxy resins, as well as in many consumer products including food containers, thermal receipts, water pipes, toys, medical equipment and electronics. The exposure to BPA, via direct ingestion, inhalation and transdermal routes can induce adverse effects on human health. BPA is a potent endocrine-disrupting compound and its epimutagenic, obesogenic and diabetogenic effects are widely reported in literature. Public concerns and government regulations on BPA stimulated the development and production of BPA substitutes. These are structurally similar chemicals to BPA, including BPS, BPF, BPAF, 4-Cumylphenol and TMBPF.

A focus of this study was to determine if BPA and its five analogues can form reactive metabolites *in vitro*. We used LC-HRMS/MS for the detection of metabolites and glutathione conjugates of these six compounds in human liver microsomes (HLM) in the presence of a NADPH regeneration system and GSH as a trapping agent. We have detected oxidation metabolites and GSH adducts in BPA and its structural analogs. HRMS/MS data was used for the investigation on fragmentation pathways of bisphenols and for the structural elucidation of metabolites.

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

Études de Triaryles Boranes dans le But d'Utilisation pour des Batteries de Types « Redox-Flow »

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Laval University

L'augmentation constante de la population provoque un besoin grandissant d'énergie pour pallier la demande. Toutefois, un des problèmes majeurs dans le domaine de l'énergie est l'incapacité d'entreposer celle-ci sur de longues périodes de temps. L'utilisation de batteries de type Lithium-ion n'est pas viable pour l'entreposage d'énergie destiné à des villes, majoritairement à cause du coût élevé de celles-ci. Une alternative intéressante est l'utilisation des batteries de type « Redox-flow » (RFBs). Ces batteries permettent de garder l'énergie en chargeant des composés électro actifs et en entreposant ceux-ci dans de grands réservoirs.

La quantité d'énergie entreposée peut facilement être mise à l'échelle en augmentant simplement la taille des réservoirs. C'est donc cet angle de recherche que nous avons emprunté, en étudiant différents composés triaryles-borane, ayant pour rôle l'anolyte dans ces batteries Leur stabilité probable face aux radicaux et leur grande fenêtre de redox en font des candidats de choix pour leur utilisation dans les RFBs. De plus, leur coût relativement faible et leur faible toxicité rendent leur utilisation d'autant plus attrayante.

N-B Bifunctionalized Polystyrene Resins as Recyclable Pre-Catalysts for the Metal-Free Borylation of Heteroarenes

N. Bouchard*, F.-G. Fontaine

Université Laval

In 2015, our group reported the catalytic metal-free borylation of heteroarenes using ambiphilic 1-TMP-2-BH_2-C_6H_4 (TMP= 2,2,6,6-tetramethylpiperidine). Since then, we reported air stable (trifluoroborate salts) and more active catalysts bearing smaller amines. The ease of synthesis of these air-stable compounds prepared from commercially available precursors paves the way to the synthesis of polymeric versions of borylation precatalysts.

We wish to report the synthesis of styrenic ambiphilic ''Frustrated Lewis Pair'' based on the *ansa*-aminoborate motif and the polymerization studies. These materials act as tunable and recyclable resins, making their implementation in flow chemistry systems easier. We will report the reactivity of these materials and highlight their potential in batch chemistry.

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

Boron Complexes of *N,N'*-Diphenylbenzamidine-*N*-Oxide Ligands with Crystallization-Induced Emission Enhancement Characteristics - Towards Blue and White OLED Applications

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N,N'-Disubstituted amidine N-oxides (AMOXs) are good chelating ligands, forming stable 5-membered chelate rings with metal ions. In addition, they present high steric and electronic modularity by structural modification of the ligand with the addition of substituents. In this work, the chemistry of $B(AMOX)Ph_2$ compounds is explored. Their synthesis and characterization are presented. The physico-chemical properties of the complexes were studied by structural analysis, computational, spectroscopic and calorimetric methods. Crystallization-induced emission enhancement (CIEE) behavior was observed and proved by the close relationship between morphology and photo-physical properties in solid state. $B(AMOX)Ph_2$ complexes are a new family of highly fluorescent small molecules and they are of interest for potential applications in optoelectronic devices (e.g., OLEDs).

Synthesis and Reactivity of Amino-Hydroborane Frustrated Lewis Pairs

E. Rochette*, F.-G. Fontaine

Université Laval

According to the longstanding definition, a frustrated Lewis pair (FLP) is the combination of a Lewis acid and a Lewis base that do not quench each other because of steric hindrance and/or geometric constraints. Since 2011, in an effort to broaden the scope of FLPs, our research group has been interested in using classical Lewis pairs that are synthetically available to effect FLP transformations. The geometrically constrained *ortho*-phenylene bridged amino-hydroboranes proved to be particularly interesting and active catalysts, notably for the borylation of Csp^2-H and S-H bonds. Moreover, a recent mechanistic study proved that despite existing as stable Lewis adducts in their ground state, less bulky analogues are more active catalysts for the Csp_2-H borylation, suggesting that the presence or absence of Lewis adducts does not always correlate to the FLP activity. Finally, while studying this reactive FLP framework, we also discovered interesting rearrangements, notably leading to the formation of a diborane and the first example of a Csp_3-H activation by a FLP. The synthesis and characterization of these new species, as well as the experimental and computational investigation of their reactivity, will be presented. distinguishes them from structurally similar and more widespread complexes, the latter more often than not being quenched by aggregation. These properties make $Al(AMOX)_3$ complexes potential candidates for OLED technology applications.

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

Ruthenium Complexes of Anastrozole as Potential Multitargeting Chemotherapeutic Agents

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INRS-Institut Armand-Frappier

Ruthenium-based complexes currently attract great attention as they hold promise to replace platinum-based drugs as first line cancer treatment: some of them i) exhibit considerable activity against cis-platin resistant cell lines, ii) induce a lower occurrence of side effects in comparison to platinum-based therapeutics, and iii) display their antiproliferative activity via different mechanisms. An appealing strategy to enhance the anticancer properties of ruthenium complexes is to design ruthenium multitasking drugs able to promote cancer cell death by various mechanisms, simultaneously. The proposed strategy could potentially lead to ruthenium complexes in which both the metal center and ligand(s) are mutually responsible for the anticancer properties of the complex. In this presentation, we report the synthesis, the characterization and the biological activity assessment of a series of ruthenium complexes in which anastrozole is coordinated the metal center. Anastrozole is an enzyme inhibitor used for estrogen receptor positive (ER+) breast cancer therapy. It is known to block the activity of aromatase, the enzyme responsible for the production of estrogens from androgens in postmenopausal women. This study opens the door to the development of a novel class of organometallic anticancer drug candidates with a broader spectrum of pharmacological activities.

Isolation of Imidazolate Borate Building Blocks and their Mechanochemical Conversion to Ultralight Imidazolate Frameworks

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Whereas metal-organic frameworks (MOFs) have emerged as the reliable go-to materials for applications requiring a tunable, multi-functional and porous system, the approaches for their syntheses still represent a number of challenges from the aspect of synthetic simplicity and efficiency, as well as the standpoint of environmental impact. Boron-imidazolate frameworks (BIFs) are a still little-known class of transition-metal or main-group MOFs that readily adopt framework topologies observed with the much more heavily studied metal azolate frameworks. A possible reason for the lesser popularity of BIFs is the multi-step and sometimes unreliable synthetic approach which involves first creating a tetrakis(imidazolato)borate anion, that is then combined with a suitable source of a monovalent main group (*e.g.* Li^+) or transition metal cation (*e.g.* Cu^+), often under hazardous conditions of solvent and temperature. This presentation outlines the first solvent-free synthesis of BIF materials, enabling the assembly of frameworks of high porosity at room temperature, from safe and readily accessible reactants, including metal oxides, hydroxides and carbonates.

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

Synthesis and Characterization of a Family of Al(AMOX)$_3$ Aluminum Complexes

H. Saavedra-Lavoie*, J. J. Castro, G. Hanan, M. Cibian

Université de Montréal

N,N'-disubstituted N-oxidized amidines' ability to form 5-membered ring complexes renders them good bidentate ligands, because this geometry offers high stability. These complexes are interesting because of the AMOX ligand's electronic modularity. Indeed, the AMOX's central carbon can don a variety of substituents varying in electron-donating and electron-withdrawing character. When complexed, these different AMOXs alter photophysical and electronic properties of said complexes. Our research lies into exploring these properties on 5 Al(AMOX)$_3$ complexes.

Synthesis of complexes and their caracterization is presented.The complexes' large visible solid state emission spectra are explored. Solvent effect on emission is also explored, offering even greater emission tuning. The complexes' aggregation induced emission (AIE)

Solid-State Routes to the Mixed-Metal Organic Mineral Paceite and its Synthetic Cadmium Analogue

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McGill University

We present syntheses of paceite, a naturally-occurring calcium copper acetate mineral, and its synthetic cadmium analogue, both entirely conducted in the solid state. Materials that contain multiple metal centres and organic ions are often difficult to prepare due to the phenomenon of incongruous solubility, where solubility differences between metal salts cause one to be preferentially deposited over the others, resulting in incomplete reactions. While conventional synthetic methodologies for these materials – those conducted in

solutions – are encumbered by this problem, emergent solid-state methods such as mechanochemistry and accelerated aging permit the rapid, precise, and efficient production of these materials without concerns related to incongruent solubility. Using the example of a cadmium-containing analogue of a copper- and calcium-based mineral paceite ($CuCa(CH_3COO)_4 \cdot 6H_2O$), we demonstrate that synthetic analogues of metal-organic minerals can be designed and subsequently synthesized by drawing inspiration not only from the composition of naturally-occurring minerals, but also from the geological processes by which they are formed.

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

Molecular Photo-Electro Catalytic System for Hydrogen Generation

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Nowadays, the conversion of solar energy into chemical bonds by water splitting is a solution for the replacement of fossil fuel [1]. The challenge consists of extracting electrons of water to form O_2 and giving electrons to protons to form H_2. In the field of molecular artificial photosynthesis, absorption, charge separation, energy transfer, electronic transfer and catalytic activity can be tuned by the chemical and structural composition of the molecules in question. To mimic the reduction part of water splitting, we use a system with a sacrificial electron donor such as triethanolamine, Ru and Ir, photosensitizer and abundant metal-based catalyst. Here we study the intrinsic properties of the photosensitizer for red shift absorption and efficiency, the tuning of cobaloxime for robustness and efficiency, and the enhancement of electronic transfer, between both entities. The association of $[Ru(L)(bipy)2]^{2+}$(L=diphenyl-[2,2'-bipyridine]-4,4'-dicarboxamide) with the new cobaltoximes shows high photo-catalytic activities. The optimizing of reaction conditions will relate the performance of each entity. Those promising property open a new door for the electro-catalytic field at the interface of materials. Herein, the synthesis, ^1H N.M.R. characterization, RX diffraction, photophysics and electrochemical measurements, and the photocatalytic activity of new species are reported.

Hypergolic Metal-Organic Frameworks as a New Class of Greener Hypergolic Fuels

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Hypergolic materials, i.e. substances that spontaneously ignite in contact with an external oxidizer, are critical components of high-energy propulsion systems required in aerospace industry. Typical propellants found in such applications are energetic hydrazine-based molecules that, while providing high combustion energies, are also extremely toxic and cancerogenic. This represents a major environmental challenge facing the modern aerospace technologies, with the atmospheric release of cancerogenic propellants estimated at over 12,000 tones in Europe alone.As a part of our research program on developing cleaner, safer and also inexpensive fuels, we now describe the very first strategy to develop microporous metal-organic frameworks (MOFs) exhibiting hypergolic behavior. This patent-pending strategy is based on introducing alkene or alkyne “trigger” groups onto the azolate linkers in popular zeolitic imidazolate framework (ZIF), a class of MOFs. By changing the node and linker components, the herein presented strategy enables access to high combustion energies and ultrafast ignition delays as low as 2 ms.

INORGANIC CHEMISTRY/CHIMIE MINÉRALE

Development of Antibiotics that are Highly Selective for N. Meningitdis and N. Gonorrhoeae

R. Vidal*, A. Castonguay

INRS-Institut Armand-Frappier

There is a need to develop novel avenues to selectively treat bacteria that are becoming increasingly resistant to currently used antibiotics. For instance, vaccines and antibiotics are currently minimally preventing a devastating global epidemic but unfortunately, some bacterial strains are rapidly evolving to escape those two types of human interventions. Notably, the two pathogenic strains of the Neisseria family are considered as an emerging public health threat. In collaboration with microbiologists from our institute, we recently found that molecules harboring a common functionality are highly effective at selectively inhibiting the growth as well as at killing Neisseria meningitidis. The aim of our study is then to develop novel a new family of antibiotics with a high activity and selectivity against the two above-mentioned pathogenic bacteria from the Neisseria family without affecting the other Neisseria that constitute the normal flora in healthy individuals. In this presentation, synthetic strategies to modify this highly selective chemical functionality as well as to introduce it into the structure of broad-spectrum antibiotics will be discussed. Results emerging from this study could lead to the development of novel strategies for the design of highly selective treatments for these two multidrug-resistant pathogens that are becoming serious human threats.

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

Computational Study of Weak Interactions in Cyclic and pi-stacked Arrangements of Model Phenolic Surfactants

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Concordia University

Lipid assemblies at interfaces possess structures that depend on their intermolecular interactions. Experimental work at the air-water interface suggests that both hydrogen-bonding and pi-stacking interactions affect the organization and behaviour of phenolic surfactant monolayers. Grazing incidence x-ray diffraction (GIXD) has yielded information on the lateral organization of the surfactants; however, the underlying noncovalent interactions remain undetermined. Modeling efforts into arrangements from electronic structure calculations in accord with the GIXD data allow the unambiguous determination of the location and strength of each noncovalent interaction.Preliminary results have been obtained for model systems using wB97X-D (density-functional theory, DFT) and GFN1-xTB (semiempirical) methods. GFN1-xTB, in particular, was specifically parameterized for noncovalent interactions and appears to be an acceptable substitute for DFT methods for larger systems. Lipid models used include *p*-alkylphenol, *p*-alkoxyphenol, and alkyl *p*-hydroxybenzoate, arranged in cyclic trimers and higher assemblies, in both the gas phase and implicit water solvent. The molecules upright themselves increasingly with lengthening alkyl tails. Our studies reveal that the predominant cyclic trimer motif evolves into a pi-stacked arrangement in larger assemblies. [1] Zhao, Y. Monolayer Behavior of Phenolic Lipids: Experimental and Computational Studies. M. Sc. Thesis, Concordia University, Montreal, QC, 2008. [2] Schmidt, R.; DeWolf, C. *Langmuir* **2004**, *20*, 3284. [3] Grimme, S.; Bannwarth, C.; Shushkov, P. *J. Chem. Theory Comput.* **2017**, *13*, 1989.

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

Component Exchange for Property Tailoring

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Component exchange is the switching of constitutional components within a given a compound. The exchange is enabled by reversible bonds. These can either be supramolecular or covalent bonds. Component exchange involving dynamic bonds can be triggered with external stimuli such as heat, catalyst or mechanical forces. It will be shown that dynamic component exchange can occur with covalent imine bonds. Property tailoring by component exchange such as fluorescence and electrochemistry is ultimately desired.

Phenyl vs. Cyclohexyl Ancillary Groups in Aminotriazine Molecular Glasses: Effect on Interaction Availability and Glass-Forming Ability

Z. Kara Ali

Université de Montréal

Aminotriazine derivatives are known to show outstanding glass-forming ability (GFA) and resistance to crystallization. The effect of various structural elements on their glass formation properties has been previously studied. However, the effect of phenyl (Ph) versus cyclohexyl (Cy) substitution as ancillary groups on the triazine's linkers at positions 4 and 6 has yet to be documented. A library of twelve compounds having a non-hydrogen bonding linker (NMe) and with different headgroups at position 2 (Et, OMe, NHMe and NMe_2), were synthesized and characterized. We found that all compounds present an outstanding GFA. Interestingly, the substitution with two Ph offers a higher resistance to crystallization. The effect of Ph versus Cy substitution on the glass transition temperature (Tg) is remarkable only in the case of the hydrogen-bonded NHMe headgroup. Variable temperature infrared spectroscopy for the three compounds with NHMe headgroups revealed that, in addition to the previously observed H-bonded and free NH groups, we can distinguish a third fraction of NH groups interacting with Ph groups. Quantification of these different NH fractions by chemometrics showed that a NH/Ph interaction hinders hydrogen bond formation and thus decreases the Tg, which is also confirmed by the calculation of dimerization constants.

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

ProDOT Derivatives: Towards Stretchable Organic Electronics

M. Lerond

Polytechnique Montreal

A series of propylenedioxythiophenes (ProDOT) were synthesized and polymerized by both chemical and electrochemical oxidation. The resulting conjugated polymers sustained electronic conduction along their backbone. This is a suitable property for using the conjugated polymers in electronic devices such as biosensors, electronic skin, OLED and photovoltaics. Owing to the solubility of ProDOT monomers in commonly used solvents, they can be copolymerized with conventionally used EDOT. Here, ProDOT derivatives were used to functionalized small elastomers prior to their crosslinking. This was to develop polymers having both electronic conduction from the ProDOT and elastomeric properties from the matrix. These properties were characterized with a stretch bench and a four-point probe station. Surface analyses by AFM and profilometry showed a interesting morphologies that will be presented.

Photo-oxidation of Langmuir Monolayers Mediated by the Hypericin Photosensitizer

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Incorporation into cell membranes is key for the action of photosensitizers in photomedicinal treatments, with hydroperoxidation as the prominent pathway of lipid oxidation. Langmuir monolayers of dioleoylphosphatidylglycerol (DOPG), 1,2-dioleoyl-sn-glycero-3-phosphocholine (DOPC), 1,2-dioleoyl-sn-glycero-3-phospho-L-serine (DOPS), and 1,2-dipalmitoyl-sn-glycero-3-phosphorylcholine (DPPC) were used as cellular membrane models to investigate the miscibility of the photosensitizer hypericin and the photo-induced effects of lipid oxidation. The Langmuir monolayers of phospholipids containing different concentrations of hypericin were made on ultrapure water subphase, characterized by surface pressure (π) - area (A) isotherms, imaging ellipsometry, Brewster angle microscopy (BAM) and surface rheology. The lipid membrane loaded with hypericin was further photo-activated to analyze the effects of lipid oxidation on the membrane properties, which included the increase of the mean molecular area for DOPG, and a decrease for DOPC. The resulting changes in the alkyl chains induced changes in the membrane viscoelastic properties which may imply different oxidations paths and products.

PHYSICAL CHEMISTRY/PHYSICO-CHIMIE

Engineering Dichroic Cocrystals Using Halogen Bonds

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The halogen bond (XB), a highly directional interaction between a halogen-atom donor and an electron-rich acceptor, has been shown to be a reliable tool for assembly of cocrystals. Most commonly forming with electronegative atoms such as oxygen or nitrogen, XBs also form with aromatic π-systems, such as in the previously described cocrystal of naphthalene and 1,4-diiodotetrafluorobenzene. Based on this, we hypothesized that replacing naphthalene by its constitutional isomer, intensely blue-colored azulene, could yield di- or pleochroic materials.

Solid-state mechanochemical methods were used to screen for and obtain halogen bonded cocrystals of azulene. Structural analysis confirmed the role of azulene as an XB acceptor, analogously to naphthalene, forming parallel XB chains with edge-to-face C−I···π XBs and giving rise to highly dichroic (blue/colorless) crystals. Varying the stoichiometry of initial components led to the ordering of azulene, while changing from 1,4-diiodotetrafluorobenzene to 1,4-dibromotetrafluorobenzene led to switching from the XB to aromatic ring stacking, significantly weakening the dichroism (blue/violet). On the other hand, replacing 1,4-diiodotetrafluorobenzene by an azobenzene-based red chromophore resulted in a blue-to-red dichroic shift.

In conclusion, we have successfully demonstrated that the optical behavior of azulene-based XB cocrystals can be tuned by changing the stoichiometry and the nature of XB donor.

Pushing the Visible Emission Envelop: Developing NIR Emitters

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Fluorophores are ubiquitous in a large range of applications such as biological imaging and organic electronics. While fluorescence in the visible region has its advantageous it is also a severe limitation. Emission in the NIR would be advantageous for both biological probes and organic emitting devices to address many of the shortcomings of visible fluorophores. Towards this means, we investigated conjugated fluorophores having an electronic *push-pull* configuration. We examined the effect of a heavy heteroatom in the core aromatic on the spectroscopic and electrochemical properties, along with the emission quantum yields. These are complemented by theoretical calculations to appreciate the fluorophore's photophysical properties.

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

Synthesis and Characterization of Liquid Crystalline Tetraoxapentacene Derivatives

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Fluorescent columnar liquid crystals could have potential applications as semiconductors in organic photovoltaic cells, field effect transistors and light emitting diodes. However, the emission of the core observed in solution is usually quenched in ordered phases.Here, the tetraoxapentacene has been studied as a core for columnar liquid crystals beacause of its emission and straighforward preparation. Our approach is to append alkoxy-substituted aryl groups to promote aggregation-induced emission (AIE) in order to exhibit fluorescence. Indeed, the energy consumed, in solution, by the rotation of functional groups in the molecule leads to a non-radiative decay. However, in solid state, the free rotation of those groups is restrained and a radiative decay (AIE) is observed.

En route to Agminosides Synthesis, Natural and Polyacetylated Glycolipids

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Agminosides are natural glycolipids isolated from the marine sponge *Raspailia agminata*, endemic of New Zealand coral reef. Since agminosides were isolated with very low yields, their biological properties have still to be deciphered. Structurally, agminosides possess a lipid chain linked to a branched hexasaccharide, which is non-stoichiometrically acetylated and composed exclusively of d-glucose derivatives connected with beta-(1–>4) and beta-(1–>2) linkages. Motivated by the atypical structure of agminosides and by the proven biological properties of structurally related marine glycolipids, we have recently undertaken their total synthesis. The structure of agminosides can be retrosynthetically disconnected into five glucose derivatives carrying preinstalled acetyl groups, and a lipid chain. This research project can be carried out according to four objectives: 1) synthesis of glycoside units by protection-deprotection; 2) stereoselective synthesis of the lipid chain; 3) one-pot glycosylation of the different units; and 4) *in vitro* studies of biological properties of agminosides and their derivatives.

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

Preparation of Alternative Nucleic Acid Structures and Evaluation of their Repair by AGT

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DNA nanotechnology, founded by Nadrian Seeman nearly 35 years ago, harnesses the Watson-Crick base pairing between complementary strands to assemble specific three dimensional structures. More recently, the use of DNA based structures for drug delivery has piqued the intertest of many nucleic acid chemists due to the versatility and cellular stability of DNA. Various approaches such as binding of small molecules or short complementary strands to trigger drug release from these DNA structures have been explored. Our laboratory is interested in evaluating the ability of the DNA repair protein O^6-alkylguanine-DNA alkyltransferase (AGT) to act as such a trigger on DNA structures for drug delivery. Recently, our group has shown that AGT has activity towards DNA containing alkylene linkages connecting the O^6-atoms of adjacent 2'-deoxyguanosine residues resulting in strand cleavage. In this study, the synthesis of an O^6-2'-deoxyguanosine-butylene-O^6-2'-deoxyguanosine nucleoside dimer for incorporation into a DNA nanostructure which may allow for efficient drug transport and mediated release by hAGT is described. The dimer was successfully prepared by a multi-step synthesis approach with moderate to good yields for each reaction. The novel compounds were characterized by ^{1}H NMR and mass spectrometry.

Synthesis of Potential Inhibitors of Bacterial Kdo-Processing Enzymes

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There is an important need for new types of antibacterial agents in present days because of the increased resistance of pathogenic bacteria. Inhibiting enzymes involved in the biosynthesis of polysaccharides from Gram-negative bacteria (GNB), such as lipopolysaccharides (LPS) and exopolysaccharides (EPS), stands as an underexplored approach to pursue. Such inhibition could ultimately lead in damaging the outer membrane of GNB.

Therefore, the objective of the research project is to synthesize Kdo mimics that could act as potential inhibitors of Kdo-processing enzymes involved in the biosynthesis of Kdo-containing LPS and EPS from pathogenic GNB. 2-Deoxy and 8-amino-2,8-deoxy Kdo derivatives along with their corresponding glycosides in both α- and β-anomeric forms have been synthesized through multi-step organic synthesis starting from d-arabinose. As a preliminary assay, Kdo derivatives have been evaluated for their ability to inhibit the formation of EPS from *Burkholderia* spp. in collaboration with the group of Prof. Éric Déziel from INRS-Institut Armand-Frappier. We showed that 2-adamantane glycosides of Kdo are able to prevent the formation of mucoid bacteria and that only the β-forms are active. Ultimately, the research project could generate novel sugar-based chemical entities, which could be used as broad-spectrum antibiotic agents against pathogenic GNB.

ORGANIC CHEMISTRY/CHIMIE ORGANIQUE

Identification of a Novel Anti-Cancer Target with Thioenoisoquinoline Derivatives

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Cancer is a leading cause of death world wide. Chemotherapies are known for their harsh side effects caused by poor selectivity for cancer cells. For this reason, the development for molecular regulators of mechanisms solely found in cancer cells is crucial for improving chemotherapies. Thienoisquinolinines are known to be an estradiol mimic and can potentially be used in the regulation of inflammation response and treat diseases related to inflammation. In preliminary studies, thienoisoquinolines show selective biological activity against cervical cancer cells. The drug candidate with a highest potency in the low nanomolar range is compound 75 (C75). This potency is selective to cells of hard to treat cancers with aberrant centrosomes over healthy cells. Further study has shown that the candidate drug prevents mitotic catastrophe in cancer cell lines that require bipolar spindle assembly in mitosis cluster. However, the mitosis clusters are found to be multipolar after C75 treatment suggesting a novel target for which anti-cancer drugs have not currently been developed. Our goal is to confirm the target of C75 and complete *in vivo* structure-activity relationship studies. Further research will continue in the pursuit of target identification and synthetic placement of a linker handle.

Partial hydrogenation of nitro to hydroxylamine group in multidentate ligands

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Catalytic hydrogenation of aromatic compounds containing a nitro group is an industrially important process for the introduction of amino functionality into pharmaceutical and agrochemical intermediates and in the polyurethane chemistry. Nitroarenes ($ArNO_2$) are easily hydrogenated, and hydrogenations have been carried out under a wide range of conditions. Formally, the reduction of nitroarene group to the corresponding amine ($ArNH_2$) proceeds via intermediate states including ArNO (nitrosoarene) and ArNHOH (hydroxylamine) species. These transformations require reduction by two electrons in each step. Herein we are interested in partial hydrogenation of NO_2 to NHOH in order to capitalize on the redox properties of the NHOH function when coordinating to a metal ion. Transition metal catalysts such as palladium, platinum, nickel and zinc are too reactive in this hydrogenation and directly convert the nitro into the amino group. To stop the reaction at the NHOH point, we used a thioether (diphenyl sulfide) poison and varied its concentration and the overall reaction time of hydrogenation keeping the other reaction conditions constant to probe its effects. Depending on a number of factors discussed above, arylhydroxylamine can build up to significant concentrations during the hydrogenation, if we reduce the time of reaction and increase the concentration of the poison. Characterization of the ensuing ligand and reaction with Cu(II) will also be presented.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Lanthanide-doped upconverting nanoparticles induce stress in mammalian cells

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Lanthanide-doped upconverting nanoparticles (UCNPs) are promising tools for cancer therapeutics because of their unique physico-chemical properties. They are commonly used in imaging and photodynamic therapy. However, their effect on living cells remains largely undefined. The exposure of cells to environmental insults, such as nanoparticles, can activate various stress responses and, at the same time, impair protein homeostasis. Stress responses often alter cell fate, which ultimately can cause cell death. These features may compromise UCNP-dependent applications in living cells. Yet, particle properties could also be explored for targeted cell killing.

Using non-transformed and cancer cells, we assessed the effects of UCNPs on cellular stress responses and nuclear trafficking. We focused on nucleoli, the compartments for rRNA synthesis, and evaluated nucleolar proteins that are required for ribosome biogenesis. UCNPs altered the abundance of several essential nucleolar resident proteins, thereby changing the overall nucleolar organization. Moreover, UCNPs diminished rRNA synthesis in cancer cells, suggesting that nucleolar function was compromised. UCNPs also affected key components that are required for transport in and out of the nucleus. Taken together, our results demonstrate that UCNPS impair rRNA synthesis and cellular trafficking. This knowledge is important for the proper development of UCNPs for cancer therapy.

Synthese of Polyserotonin Nanoparticles for Anti-Bacterial Applications

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In the last few decades, the rate at which microbes develop resistance has outpaced the development of new antibiotics. As a result, there is an urgent need to discover and/or design alternative therapeutics with improved efficacy without conferring further resistance is on demand. This research exploits the use of polyserotonin nanoparticles (PSeNPs) as a platform to target bacterial adhesion and biofilm formation—a key contributor to bacterial resistance. Recently, PSeNPs have been shown to be effective anti-cancer therapeutic agents owning to enhanced resistance to protein corona, high biocompatibility, and utility in photothermal capabilities. We aim to harness the unique properties of PSeNPs by modifications on the surfaces to target bacterial cells. Herein, we compare two different synthetic routes of PSeNP formation—via aqueous (phosphate buffer) and water-alcohol mixture—using UV-vis spectroscopy to monitor its synthesis, scanning electron microscopy (SEM) for size distribution, and fourier-transform infrared spectroscopy (FTIR) to confirm structural information. Our preliminary data shows that both aqueous and water-ethanol mixture generated PSeNPs where the latter results an improved monodispersity of nanoparticles. Ultimately, PSeNPs from each synthetic route was further functionalized with polyethylene glycol (PEG) which will be explored to evaluate the alteration capabilities to target biofilms.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

GATA4-Mediated Gene Expression Promotes Muscle Remodeling During Stress in the Freeze-Tolerant Wood Frog, *Rana Sylvatica*

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The wood frog, *Rana sylvatica*, can withstand full body freezing in winter, where over 70% of its total body water is converted to ice. Frozen wood frogs show no signs of brain conductivity, heart beat, breathing, or muscle movement for months at a time, but return to full function once thawed. Freezing is accompanied by dehydration, anoxia, and hyperglycemia; the latter caused by overproduction of glucose to be used for cryoprotection. As such, wood frogs must overcome numerous biochemical and physiological stresses to survive freezing. GATA4 and Nkx2.5 are two transcription factors that promote muscle remodeling and cardioprotection by regulating the expression of key downstream genes (troponin I and C) during stress. This study examined the effects of freezing, anoxia, and dehydration on the expression levels of GATA4 and Nkx2.5 transcription factors along with selected downstream genes in the skeletal and cardiac muscle of wood frogs. Overall, our results show that GATA4 and Nkx2.5 are regulated in a tissue and stress-dependent manner. Exposure to freezing and anoxia caused an overall decrease and increase in GATA4 mediated-transcription in cardiac muscle, respectively. In skeletal muscle, exposure to anoxia caused a decrease, whereas freezing and dehydration had no overall effects on GATA4 transcription.

Effect of Binding Interference on the Divergence Between Paralogous Genes Encoding Homodimers

A. F. Cisneros[*], H. A. Jain, C. R. Landry

Laval University

The physical association of proteins is a key process that constrains a protein's evolution to the sequence space that can maintain its interactions with other proteins. Duplication of genes encoding homomeric proteins gives rise to another identical homomer and a heteromer. This phenomenon, called "paralog interference", can lead to dosage imbalance due to the excess in complex activity. However, it can be solved by divergence between the paralogs. The retention of specific complexes allows them to split the ancestral functions or even develop new functions. It is our objective to study how the evolution of paralogs can influence the retention of these interactions. By means of simulations, we evaluate the binding energy of the complexes as the paralogs accumulate mutations under different selection scenarios determined by specific fitness functions. As a large fraction of genes encode homomeric proteins, the resolution of paralog interference is an important factor in the evolution of protein-protein interaction networks.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Torch Protein Library

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To understand how any living system functions, one inevitably has to know the three-dimensional structure of a large number of proteins. Despite the recent progresses in cryo-electron microscopy, experimental approaches to this problem are unlikely to scale up, and there is a dire need for innovation in computational methods. State-of-the-art methods that attempt to solve the protein folding problem usually rely on complex workflows that consist of multiple loosely interconnected operations. However, new computational approaches to protein folding have recently emerged, which make use of end-to-end learning. We anticipate that end-to-end models will become extremely important for structural biology,

due to the growing amounts of data for both protein sequences and protein structures, and the necessity of relating the two. Since the transformation between internal coordinates and atomic positions is the only known unambiguous differentiable mapping between protein sequence and protein structure, we also believe that fast implementation of this transformation will be a key building block for all sequence-to-structure models. In this work we present TorchProteinLibrary, a library that implements the conversion between internal protein coordinates and atomic positions for ``full-atom" and ``backbone-only" models of protein structure.

OCT Induced Transcriptional Network in the Freeze-Tolerant Wood Frog

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Carleton University

Wood frogs, *Rana sylvatica*, have the remarkable ability to withstand whole body freezing during the winter. Freezing induces metabolic, oxidative, biochemical, and physical stress as the animal undergoes dehydration, anoxia, ischemia and hyperglycemia. These cellular stresses can all lead to increased oxidative stress, potentially initiating destructive pathways such as apoptosis. Octamer Transcription factors (OCT) are highly conserved gene regulatory factors that bind to an 8bp consensus DNA sequence (‘5-ATGCAAAT-3’ (the octamer motif)). Eleven OCT isoforms are known with OCT1, 2 and 4 being prominent members that have been widely studied with respect to their roles in stem cells, embryonic stages and adult tissues. OCT1 and OCT4 are potent stress responsive transcription factors, particularly involved in oxidative stress and antioxidant defense. The present study examines the responses of OCT1, OCT2 and OCT4 during freezing and thawing in different tissues (Brain, Heart, Liver and Kidney) of wood frogs as well as selected group of their downstream targets. Significant changes were seen in different treatments (frozen and thaw with respect to control) of brain and heart where as maximum expression of all OCTs were observed in frozen liver and frozen muscle.

In Silico Study of Epistasis in Protein Protein Interactions

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Laval University

Epistasis, an important phenomenon observed in evolution, describes the effect of one mutation on other. It has been shown that the combined effect of a series of mutations on a protein is different from the sum of the effects of the individual mutations. Here, we are studying the phenomenon of epistasis in protein-protein interactions using an *in silico* model for yeast paralogs after the event of gene duplication. Duplication of a gene whose encoded protein forms homodimers by interacting with itself gives rise to three complexes: two homodimers and a heterodimer of paralogs. Mutations play an important role in determining the retention or loss of these complexes. Our focus lies on studying these mutations present in the interface region of the paralogs, analyzing the effect of order of mutations and finding specific residues which have a major effect on the binding energy of complexes. These simulations can be further extended to finding relevant residues for efficient protein design.

Peroxiredoxin Expression in the Wood Frog, *Rana sylvatica* in Response to Freezing

Z. Lung*, K. Storey

Carleton University

The wood frog (*Rana sylvatica*) has developed a winter survival strategy that involves whole body freezing on the forest floor and drastically reducing its metabolic rate. In order to protect their cells while experiencing this stress, *R. sylvatica* strongly elevates its glucose levels (from 5mM to 300mM) and uses glucose as its cryoprotectant through the winter. In the frozen state, wood frogs must additionally endure anoxia and dehydration stresses on its cells as well as dealing with stress due to reactive oxygen species. Therefore, adequate antioxidant defences are critical to maintaining cell viability over freeze/thaw cycles. Peroxiredoxins (Prdx) are a known, ubiquitous family of proteins involved in antioxidant defence and also induce various cellular stress defences. Using *R. sylvatica* as the animal model allows for expanded knowledge of how this family of antioxidant proteins function amid stress. The focus of this project is to analyze the peroxiredoxin family protein expression (Prdx 1- Prdx 6) to freezing stress using SDS-PAGE to evalaute *R. sylvatica* liver, muscle and brain.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Exploring Stress Granule Formation in Senescent Kidney Cells

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Organ functions decline during aging, and the most profound changes occur in the kidney. Kidneys are continuously exposed to oxidative stress. They are particularly vulnerable to physiological and environmental damage. The proper response to stress is crucial for cell and organ survival. To survive different forms of insult, eukaryotic cells form cytoplasmic stress granules (SGs). This process is conserved among divergent species**.** Aging impairs the stress response, but little is known about the underlying mechanisms. It is our goal to define how aging compromises the kidney's ability to cope with stress. To this end, we developed two models of renal proximal tubule cell aging. They are based on the chemical or pharmacological induction of senescence. We demonstrated that both model systems display hallmarks of aging. Using these models, we assessed SG formation and stress-induced signaling. We showed that aging impairs SG assembly. Moreover, our studies uncovered and characterized the underlying mechanisms at the molecular level. Taken together, our research provides a better understanding of the senescence-dependent changes in kidney physiology. We identified new biomarkers that can score the stress response in kidney cells. Long-term, this information will help to develop new diagnostic and therapeutic tools to evaluate cellular aging.

Study of Localization and Function of Cep44

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Centrosomes are the microtubule-organizing centers (MTOC) in animal cells and play a significant role in maintaining cell shape, cell motility and cell polarity. During mitosis, centrosomes establish the poles of mitotic spindles that separate replicated chromosomes in dividing cells, hence playing a crucial role in cell division. Centrosomal abnormalities have been observed in tumors, microcephaly, and a number of genetic diseases such as eye and kidney diseases. Human centrosomes are composed of hundreds of proteins, but the biological functions of these proteins in organelle biology are not fully understood. Here, we began to characterize centrosomal protein of 44kDa (Cep44), acentrosomal protein identified in a proteomic analysis of the human centrosome. Cep44 localizes to the centrosome in the G0, G1, S and G2 phases of the cell cycle but it becomes less concentrated at the centrosome in the mitotic phase, suggestingthat this protein may carry out an important, but as yet unidentified, function during interphase. Furthermore, Cep44 localizes to the proximal region of centrioles where it may participate in centrosome cohesion, centriole cohesion, and/orrootlet formation. Future studies will determine the precise biological function of Cep44 and whether or not it is deregulated in human disease.

MOLECULAR BIOLOGY/BIOLOGIE MOLÉCULAIRE

Gene Regulation During Hypometabolism - Coping with Environmental Stress

K. Storey

Carleton University

Our research program is aimed at discovering the cellular and molecular mechanisms that allow both vertebrate and invertebrate extremophiles to cope with extreme environmental stresses including freezing, oxygen deprivation and winter hibernation. Our specific interests include gene regulation response to metabolic rate depression, a global method to suppress metabolic costs and prolong life under stress conditions. Areas of research include: epigenetics, post-transcriptional modifications, and microRNA regulation.

Identification and Investigation of Novel IRES Trans-Acting Factors Found to Nonspecifically Regulate Multiple Eukaryotic IRES Elements

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Carleton University

In eukaryotic cells protein biosynthesis can be initiated through secondary structural elements within mRNA called internal ribosome entry sites (IRES). This alternative translation pathway is mediated by direct recruitment of ribosome to specific regions in association with IRES *trans*-acting factors (ITAFs). It is assumed that IRES-mediated mechanism facilitates initiation of translation under conditions which impede the proper progress of cap-dependent mechanism In current study, we identified potential novel genes encoding different ITAFs. We conducted a high-throughput plasmid-based screening using *Saccharomyces cerevisiae*. This involved constructing 12 plasmids each containing a different eukaryotic IRES element fused to a *β-galactosidase* reporter cassette. Four of these constructed plasmids showed constitutive IRES-mediated expression which lead to primary identification of 142 gene candidates out of 4300 gene knockout stains. 5 candidate genes with potential role in IRES-mediated translation were selected for further investigation due to their involvement on three or more IRES elements. Quantitative β-galactosidase assays showed lower level of expression for all corresponding IRES elements in the absence of these genes. RT-qPCR analysis was performed to confirm consistency of mRNA content. In conclusion, it seems that selected candidate genes are potentially involved in cap-independent translation, by playing a role as ITAFs.

m6A Methylation Alters Translational Activity during Hibernation in a Small Mammal, the 13-Lined Ground Squirrel.

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Carleton University

As winter approaches some small mammals lower their metabolic rate and enter hibernation to survive seasonal stresses including extreme cold and limited food availability. Hibernation is a drastic mechanism for surviving harsh winter conditions in small mammals, allowing conservation of about 90% of the energy normally required to remain active as body temperature falls to near ambient and metabolism relies on stored body fats for days or weeks. For the thirteen-lined ground squirrel (13LGS), *Ictidomys tridecemlineatus*, significant reductions in metabolic rate and physiological parameters take place, as cells rapidly redirect fuel to maintaining regulatory mechanisms. Namely, global controls on both transcription and translation are implicated in the transition. In comparison to methylation of DNA or proteins, mRNA methylation is nearly uncharted territory. Methylation of Adenosine (m6A) occurring on nitrogen-6 of the basic group is shows tissue-specific differences and is associated with multiple effects on mRNA transcript stability and translational activity. Significant and tissue-specific changes in enzymes that methylate mRNA and proteins that bind m6A-laden transcripts were observed across several time-points of the hibernation cycle, showing their intricate regulation during this cellular stress. The data presented here raise the possibility that mRNA methylation plays a regulatory role in hibernation.

Enrichment of Oxidized Peptides Allows Identification of Oxidized Cysteine Residues in Signaling Proteins *In Vivo*

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Detection of oxidative post-translational modifications (ox-PTMs) of Cys residues in mammalian signaling proteins *in vivo* is one of the current challenges in redox biology. Ox-PTM residues labeling using switch methods coupled to mass spectrometry (M/S) or immunoblot have rendered possible the identification of signaling proteins subjected to ox-PTM. However, the low sensitivity remains a major hurdle to the detection of the modified residue(s) for the low abundant less reactive proteins. Here, we report a modified method of ox-PTM protein labeling coupled to M/S that highly improved the enrichment of oxidized peptides and the identification of specific ox-PTM Cys residues *in vivo*. In cell lines treated with diamide, a thiol-oxidizing agent, or HOCl, we identified 2699 peptides, covering 1473 proteins, containing at least 1 ox-PTM Cys residue. Previously reported ox-PTM residues were confirmed *in vivo*, validating our approach. Signaling proteins, including kinases, phosphatases and translation factors are largely represented. Altogether, the use of an improved method with higher sensitivity for the detection of ox-PTM Cys residues *in vivo* allowed us to deepen our understanding of redox signaling. Network analyses allowed us to highlight signaling pathways enriched in oxidized proteins related to innate immunity, antiviral response and inflammation.

BIOCHEMISTRY/BIOCHIMIE

New Investigation of Mannose Lipid in Peptide Drug Development

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Many individuals struggle to quit smoking due to nicotine addiction. Using a kappa opioid receptor (KOR) antagonist, we hope to block the cycle of addiction that causes individuals to relapse.

The use of peptides as KOR antagonists is becoming more important in drug development due to their generally low toxicity. However, the therapeutic potential of peptides is limited due to their low bioavailability *in vivo*. The purpose of this research was to increase the stability of KOR antagonist peptides in human plasma using a C_{14}-alkyl-mannopyranoside delivery system, developed by our group in collaboration with Dr. Roy and Dr. Schiller's lab. RP-HPLC was used to study the stability of the KOR antagonist, dynantin peptide. Subsequently, the *in vitro* Parallel Receptor-ome Expression and Screening via Transcriptional Output–Transcriptional activation following arrestin translocation (PRESTO-TANGO) system was used to study the affinity of dynantin at the KOR. Our results show that peptide entrapment and stability was significantly enhanced when the mannose-lipid delivery system was used with increasing ratios of Dynantin: Mannose Lipid: Cholesterol. Also, the delivery systems caused no effect on the affinity of dynantin at the KOR. This delivery system also shows a promising ability to increase peptide stability in vaccine development.

Quantification of Proteins in Solution *via* Ultraviolet-Induced Reactions of 2,2,2-Trichloroethanol with Tryptophan and Tyrosine Residues

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Protein quantification is a crucial aspect of many molecular biology and biochemistry workflows, often required for comparisons between samples. Common protein quantification assays utilized in biochemistry and molecular biology include, but are not limited to, 280 nm absorbance measurements, the Lowry assay, the Bradford method, as well as modifications of the latter two. These assays provide convenience such that they can be performed in a microplate or cuvette format, reducing procedural complexity. Previously described, 2,2,2-trichloroethanol (TCE) can be included in SDS-PAGE gels, allowing for protein quantification for a limited number of samples after a time frame greater than 45 minutes. Herein, we have developed the first fluorescent microplate-based protein quantification assay to utilize TCE. Ultraviolet (UV) irradiation induces the reaction of TCE with tryptophan and tyrosine residues, yielding redshifted excitation and emission spectra of proteins. The microplate-based TCE assay reduces the procedural time to less than 10 minutes, requires a fraction of reagent than the SDS-PAGE format, was capable of quantifying greater amounts of protein than the aforementioned assays, and was demonstrated to be useful for the quantification of protein in cell lysates.

BIOCHEMISTRY/BIOCHIMIE

Regulation of the TCA Cycle Through Modification of the α-Ketoglutarate Dehydrogenase Complex in a Mammalian Hibernator, the Richardson's Ground Squirrel (*Urocitellus Richardsonii*)

S. Green*, K. Storey

Carleton University

The TCA cycle is a central metabolic pathway serving as a hub linking carbohydrate, lipid and amino acid metabolism in the mitochondria. The α-ketoglutarate dehydrogenase complex (αKGDHC) consists of three enzymes that together catalyze the rate-limiting step of the TCA cycle through the transformation of α-ketoglutarate to succinyl-CoA. Richardson's ground squirrels (*Urocitellus richardsonii*) greatly reduce body temperature (to as low as 2°C) and basal metabolic rate (BMR) to just 1-5% of normal when they enter hibernation. The current study assessed multiple properties of αKGDHC partially purified from skeletal muscle of euthermic versus hibernating ground squirrels. The results showed a significantly increased K_m value for CoA by αKGDHC from skeletal muscle of hibernating animals at 5°, 22° and 37° C (2.39-3.26 fold increase) and the K_a of Ca^{2+} was also noticeably higher at 5° C than at other temperatures (about 2.3 fold higher). Immunoblotting revealed an increase in tyrosine phosphorylation of the three αKGDHC enzymes during hibernation. Taken together these results suggest that regulation of αKGDHC effects a reduction in activity consistent with the reduced metabolic state that occurs in hibernation and that this is maintained by posttranslational modification of KGDHC during hibernation and is also influenced by low temperature.

SUMO Site- and Paralog-Specific Identification by Mass Spectrometry

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Université de Montréal, Institute for Research in Immunology and Cancer

SUMOylation is a post-translational modification (PTM) that involves the addition of a small ubiquitin-like modifier (SUMO) protein to a substrate protein. Like many PTMs, SUMOylation has been characterized as an essential mechanism in the regulation of numerous cellular processes; including, transcription and the cell cycle. In mammals, three SUMO paralogs (SUMO1-3) are present in all cells; however, their distinct functional roles remain elusive. To better understand the unique roles of SUMO-paralogs, we sought to identify site- and target-specific modifications by SUMO1 and SUMO3 in human cells treated with the proteasome inhibitor MG132. Our proteomic approach combines molecular biology, affinity chromatography and mass spectrometry to enrich and analyze proteins modified by SUMO. By implementing this approach, we identified 6881 sites on 2102 proteins modified by SUMO1, and 10552 sites on 2995 proteins modified by SUMO3. Preliminary analysis of the data indicates several distinct protein domain enrichments between SUMO1- and SUMO3-modified proteins. Our SUMO remnant immunoaffinity purification approach has been successfully applied to the isolation of substrates preferentially modified by SUMO1 and SUMO3 (such as RanGAP1 and PML respectively) and provided information on the modification site. Additional information on the roles of SUMO1/3 will be uncovered as our data is further analyzed.

BIOCHEMISTRY/BIOCHIMIE

Investigating New Roles for Cytochrome C Peroxidase (Ccp1) in Antioxidant Defense Using its M172a Variant

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From studies in yeast, it has been shown that Ccp1 acts as an H_2O_2 sensor rather than an H_2O_2 scavenger. Oxidation of Ccp1 by H_2O_2 in respiring mitochondria converts it into a sensor of peroxide stress. This involves oxidation of its heme ligand (H175) and labilization of its heme, which is recruited for apo catalase maturation. We hypothesize that neighboring M172 promotes oxidation of H175, so we are examining the M172A and M172S variants. Alanine substitution gives an inert side chain at position 172 that is non-bulky but retains the secondary structure preference of its environment. The M172A variant has been overexpressed and purified from *E. coli* cells. Following reconstitution with heme, holoCcp1(M172A) and wild-type Ccp1 were oxidized with 1-10 molar equivalents of H_2O_2, digested with trypsin, the peptides were desalted on C18 Ziptips and analyzed by mass spectrometry. The MS spectra reveal different patterns of heme-mediated residue oxidation in the two Ccp1 variants. Notably, H175 oxidation is detected in neither variant but M172A is less oxidized than WT Ccp1. Thus, we confirm that M172 influences hole (radical) hopping away from Ccp1's heme in vitro but we still need to confirm its role in cells.

Biophysical Analysis of Heme Binding to Human Glyceraldehyde-3-Phosphate Dehydrogenase

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Glyceraldehyde-3-phosphate dehydrogenase (GAPDH) is an essential enzyme known for its role in the glycolytic pathway for catalysing the conversion of glyceraldehyde-3-phosphate to 1,3 bisphosphoglycerate in the presence of NAD^+ and inorganic phosphate. However, recently GAPDH also has been shown to deliver heme to certain proteins like NO synthase, that require it to carry out its functions. We are systematically exploring the heme binding property of human GAPDH (hGAPDH) using various spectroscopic techniques (UV spectroscopy, circular dichroism) and subsequently comparing the results with that of rabbit muscle GAPDH which is being used as a reference hemoprotein. After successfully transforming BL21(DE3) cells with pET15b encoding for N terminally his-tagged human GAPDH, the protein was overexpressed under optimum conditions and purified. hGAPDH after his tag cleavage was then used for subsequent heme binding studies. Although the spectroscopy analyses are still ongoing, preliminary titrations of heme and hGAPDH using UV spectroscopy have showed negligible/non-specific binding between heme and hGAPDH thus contradicting existing literature which indicates otherwise. Further studies will be used to confirm the negligible interaction between the two.

BIOCHEMISTRY/BIOCHIMIE

Mondo A: A Key Regulator of Sugar-Induced Gene Expression in Frozen Wood Frogs, *Rana Sylvatica*

G. Singh

Carleton University

The wood frog can survive up to 70% of whole body freezing during winter but return to full functions, unharmed, after thawing. These animals accumulate large quantities of cryoprotectants, mainly glucose to prevent architectural damage due to ice crystal formation and dehydration.

Their blood glucose levels rises from 5mM to 300mM under normal to freezing conditions. Wood frogs reorganize their metabolism so that the enough energy is available for pro-survival mechanisms. Mondo A is a glucose responsive transcription factor, that interacts with MLX to induce the expression of several downstream targets in response to the rise in glucose levels. It plays a role in insulin resistance and is deemed as target to prevent type-2 diabetes in preclinical trials. This study investigates the effects of freezing on the regulation of the Mondo A-induced transcriptional network in the wood frogs. Preliminary results suggest that MondoA protein levels are induced in both liver and brain of frozen wood frogs; thereby leading to the induction of selected downstream targets. TXNIP, a downstream target of MondoA was shown to be highly induced in both tissues, showing its role in promoting insulin resistance. This allows wood frogs to retain high blood glucose and survive in cold.

Novel Research - Biochemistry and Molecular Biology of Environmental Stress

K. Szereszewski*, H. Hadj-Moussa, A. Watts, K. Storey

Carleton University

Our research program is aimed at discovering the cellular and molecular mechanisms that allow both vertebrates and invertebrate extremophiles to cope with severe environmental stresses. Our specific interests include gene regulation responses to metabolic rate depression. Novel areas of research include microRNA regulation in new and interesting animals, novel neuronal mitochondrial peptide regulation, as well as the circadian rhythms of hibernators.

ENVIRONMENTAL CHEMISTRY/CHIMIE ENVIRONNEMENTALE

A Non-Target Workflow for the Identification of Trace Organic Contaminants Using LC-MS/MS

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Analysis of trace organic contaminants such as industrial chemicals, surfactants, cosmetics, pharmaceuticals and pesticides in surface waters is in the middle of a paradigm shift. Non-target screening (NTS) is rising in popularity due to the limitations of target analysis. Such limitations include the need of reference standards that are not always commercially available. However, reliable identification with NTS remains a difficult process as processing tandem mass spectrometry (MS) data remains a time-consuming task and the use of online libraries is limited by the number of compounds with available high-resolution tandem MS spectra. To address those shortcomings, a new workflow using a cloud-based algorithm to perform a computational library search was developed and evaluated in a blind test study. Over 60% of the spiked compounds were correctly identified at concentrations in a 50-100 ngL^{-1} range. The workflow was then used to identify trace organic contaminants in the Magog River in Sherbrooke. Compounds such as the octoxynol family of surfactants, polyethylene glycols chains of various length. Other pharmaceutical and surfactants and flame retardants were also found.

Benign by Design and by Synthesis: Mechanochemical Solvent-Free Synthesis of Edible MOFs

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Metal-organic frameworks (MOFs) are porous materials constructed from organic linkers and metal-based nodes. MOFs have been extensively studied due to their modular nature which permits functionalization of organic linkers and variation of the nature of the metal centre, thereby widening their application in many areas, including catalysis, separation, and drug delivery. However, MOFs are often synthesized from components that are not biocompatible, raising the need to develop precursors that are safe, based on food-grade materials. Cyclodextrins (CDs), cyclic oligosaccharides derived from starch, are a viable alternative to traditional MOF linkers. While MOFs based on g-CD are readily prepared from solution, such routes are environmentally taxing. Here, we present the first solvent-free routes to such “edible MOFs”, based on γ-CD units and mono- and divalent main group cations, such as Rb^+, K^+, Na^+, Cs^+, Mg^{2+} and Ca^{2+}.

ENVIRONMENTAL CHEMISTRY/CHIMIE ENVIRONNEMENTALE

The Development of a Model to Predict the Viscosity of Atmospheric Aerosols

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Aerosols are submicron-sized particles that are emitted into the atmosphere by biogenic and anthropogenic sources, or they form in the atmosphere due to chemical transformations of gaseous precursors. They impact global climate by interacting with solar radiation and acting as cloud nuclei. It was long believed that aerosols were either well-mixed, liquid droplets (if they absorbed water vapour from the surrounding air) or crystalline solids. Evidence has since emerged suggesting that aerosols can also exist in semi-solid or glassy states. Understanding the phase state of aerosols is crucial for accurately quantifying their lifetimes and their ability to act as ice cloud nuclei. To this end, this project involves developing a thermodynamics-based model to predict the viscosity of aerosols. Thus far, the model has been trained with viscosity data for a dozen lab-made, surrogate aerosol mixtures. Now the model is being tested for its ability to predict the viscosity as a function relative humidity, temperature, and composition of chemically complex, "natural" aerosols. Future work will involve using the Stokes-Einstein relation to translate the model's viscosity predictions into molecular diffusion constants for the aerosol. As such, kinetic transformations of the aerosol can be quantified from its material property of viscosity.

Removal of Pharmaceuticals in Hospital Wastewaters by Wet-Air Oxidation

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Traces of pharmaceuticals are present in many environmental waters and hospitals are major contributors to this issue. Since conventional water treatment technologies are not adequate to remove these organic contaminants from effluents, several treatments have been proposed such as ozonation and advanced oxidation processes. This project focuses on the application of a wet air oxidation (WAO) process for the treatment of hospital wastewaters before they reach municipal wastewaters. Eighteen pharmaceuticals have been selected for this study according to ecotoxicological and pharmaceutical consumption data. An liquid chromatography-tandem mass spectrometry method has been developed to quantify these problematic compounds. The validation of the method (precision: 1-22 %, accuracy: 0.2-23%, LOQ: 0.2-16 µg/L) demonstrated that it works well for most of the target compounds. Preliminary results of WAO with the selected compounds at different temperature and oxidation time will be presented. Ecotoxicological tests with *Daphnia magna* showed significant difference ($p > 0.05$) for day 7 and 11 between control and exposed individuals at 1 µg L^{-1}. However, there was no difference for the concentration of 20-hydroxyecdysone (possible toxicity biomarker). Furthermore, a significant increase in fecundity was observed at 6 µg L^{-1} from day 9 until the end of the test.

ENVIRONMENTAL CHEMISTRY/CHIMIE ENVIRONNEMENTALE

Study of the Occurrence of Trace Organic Contaminants in Eastern Canadian Lakes

L. Lahens*, A. Dion-Fortier, H. Cabana, P. Segura

Université de Sherbrooke

Trace organic contaminants are mostly studied in rivers and wastewater, but data is lacking on their presence and concentrations in lakes. These contaminants can be persistent organic pollutants, such as pesticides, as well as contaminants of emerging concern, such as pharmaceuticals, personal care products and industrial additives. Here, we present a multi-residue method developed to quantify 50 contaminants. This method will be applied to evaluate the contamination of around 300 lakes, representative of the distribution of lakes in Canada regarding ecozones, size and human activities impact, sampled over the country within the Lake Pulse Network. The molecules of interest will be extracted from lake water by solid phase extraction (SPE) before being analysed using ultra performance liquid chromatography coupled to triple quadrupole mass spectrometry (UPLC-QqQMS) in positive or negative electrospray ionisation. The method's figures of merit, such as the SPE recoveries (49 – 105%), method detection limits (13 – 294 ng/L), precision (2 – 33%) and accuracy (1 – 25% for most compounds) will be presented. First results on the contaminants concentrations in around a hundred lakes show that at least one compound was identified in 70% of the lakes. The link between contamination and land use will be discussed.

Method Development for Trace-Level Quantification of Nitrosamines in Wastewater

A. Lapointe*, S. Gallant, S. Comtois-Marotte, K. C. Waldron, A. Furtos

Université de Montréal

Regenerable aminated solvents used for CO_2 capture, for example piperazine, undergo degradation over time forming nitrosamines such as nitrosopiperazine. These compounds are eventually released in wastewater where their concentration should not exceed 1 ppb to respect environmental regulations. Our group was asked to develop a procedure to quantify two nitrosamines in wastewater by Liquid Chromatography-Mass Spectrometry (LC-MS). Wastewater is a complex matrix so to achieve the best limits of quantification (LOQ), sample treatment by immobilized liquid/liquid extraction (ILLE) was chosen to clean up the sample. In initial experiments, where a deuterated internal standard was used for calibration curves, an abnormally high recovery (> 200%) for ILLE-LC-MS was observed when analysing real samples spiked before and after extraction. We soon realized the standard samples had to be prepared in a high-salt synthetic matrix to mimic the real sample matrices which allowed us to achieve more realistic recoveries by ILLE. In addition, the drying steps after extraction were optimized. Separation of the highly polar analytes was achieved using a HILIC (hydrophilic interaction chromatography)-based separation on an XBridge Amide stationary phase. The triple quadrupole MS was operated in positive electrospray and multiple reaction monitoring (MRM) mode, which provided an LOQ of 0.25 ppb.

NANOCHEMISTRY/NANOCHIMIE

Influence of Nucleotide Modifications at the C2′ Position on the Hoogsteen Base-Paired Parallel-Stranded Duplex of Poly(A) RNA

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Polyadenylate (poly(A)) has the ability to form a parallel duplex with Hoogsteen adenine:adenine base pairs at low pH or in the presence of ammonium ions. In order to evaluate the potential of this structural motif for nucleic acid based nanodevices, we characterized the effects on duplex stability of substitutions of the ribose sugar with 2′-deoxyribose, 2′-*O*-methyl-ribose, 2′-deoxy-2′-fluoro-ribose, arabinose and 2′-deoxy-2′-fluoro-arabinose. Deoxyribose substitutions destabilized the poly(A) duplex both at low pH and in the presence of ammonium ions: no duplex formation could be detected with DNA poly(A) oligomers. Arabinose and 2′-deoxy-2′-fluoro-arabinose nucleotides strongly destabilized poly(A) duplex formation. In contrast, 2'-*O*-methyl and 2′-deoxy-2′-fluoro-ribo modifications were stabilizing either at pH 4 or in the presence of ammonium ions, respectively. The differential effect suggests they could be used to design molecules selectively responsive to pH or ammonium ions. To understand the destabilization by deoxyribose, we determined the structures of RNA poly(A) duplexes with a single DNA residue by NMR spectroscopy and X-ray crystallography. The structures revealed minor structural perturbations suggesting that the combination of sugar pucker propensity, hydrogen bonding, pKa shifts, and changes in hydration determine duplex stability.

Developing and Integrating Donor Chromophore Acceptor (D-C-A) Assemblies onto Semiconductor Surfaces to Drive Single Electron Transfer Processes

Z. Singh*, M. B. Majewski

Concordia University

Satisfying world's energy demand using solar energy by converting and storing it into chemical bonds is one of the most useful phenomena borrowed by humans from nature. However, oftentimes, systems that perform this solar-to-chemical energy conversion are costly, inefficient, and require the use of toxic elements. Herein, we focus on modifying the known techniques for synthesizing and integrating systems which can harvest solar energy and use it to drive fuel forming transformations. For this purpose, we describe a strategy for making films of Cu(I) single electron transfer(SET) donor-chromophore-acceptor(D-C-A) system in which the photon absorption may give rise to a long lived charge transfer(CT) state in high quantum yield. We anticipate this CT state will be populated by the donor moiety and depopulated by attached electron acceptors. This carefully constructed system will act as an electron transfer cascade to transfer a single electron which can then be used by a proton reduction catalyst to generate hydrogen or simply as an exciton in solar cells. Furthermore, the developed D-C-A assembly can be coupled to semiconductor surface to generate a dye sensitized photo electrochemical (DS-PEC) system using a bottom up approach and can further be fabricated into device.

NANOCHEMISTRY/NANOCHIMIE

Residual Chirality in Carbon Dots from Enantiomers of Amino Acids

F. Victoria*, R. Naccache

Concordia University

Carbon Dots (CDs) are one of the new members in the carbon nanoparticle family. They are primarily composed of amorphous sp^2 carbons with sizes ranging within 10 nm. These nanoparticles have demonstrated excellent tunable fluorescence, low toxicity, chemical inertness and biocompatibility. These versatile properties of CDs are determined by the starting materials and they can be synthesized from various carbon sources and passivating agent. As such, we are interested in exploring residual chirality in these carbon nanomaterials by starting with chiral amino acid precursors. This is due to the fact that chirality has been very important in pharmaceutical research for drug development and design, as well as in applications of organocatalysis, enantioselective recognition and chiral sensing. We report a facile, one-step microwave-assisted synthesis of chiral CDs from both enantiomers of cysteine, serine, and alanine.

Visible-Light Sensitization of Inorganic Semiconducting Nanostructures for Photoelectrochemical Energy Conversion

F. Yarur Villanueva*, M. B. Majewski

Concordia University

The detrimental effects of the use of fossil fuels have brought about the need to develop sustainable and renewable energy technologies to supply the energetic demands of a carbon-neutral society. Converting solar energy into chemical fuels (i.e. artificial photosynthesis) and industrially relevant chemicals or organic compounds is an attractive alternative to address the global energy problem. Artificial photosynthetic systems require, amongst other things, a high stability under continuous light irradiation and the use of Earth-abundant elements to make these technologies economically feasible. The use of metal oxide nanomaterials as semiconductors has attracted significant attention within the past few decades due to their stability, low cost, high surface area, and ability to absorb light from different parts of the solar spectrum. However, the use of these materials for artificial photosynthesis is partially hindered by their limited absorption range in the solar spectrum and high rates of electron recombination within the material. In this work, we explore options to maximize the light harvesting properties of zinc oxide nanowires and how to minimize electron recombination while using different solar fuels co-catalysts.

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We hope you had a wonderful experience at the 21st iteration of the CBGRC and we look forward to seeing you all again next year!

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Nous espérons que la CBGRC 2018 fut une expérience très agréable. Nous souhaitons avoir le plaisir de vous revoir l'année prochaine!

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