

# Abstracts

## Conformation Dynamics of Keap1 Reactive Site Cys151 Changes due to Electrophilic Influences

**Archita Adluri (Memorial University of Newfoundland)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CATC best overall oral presentation in Theoretical Chemistry

Division: Undergraduate Physical, Theoretical, and Computational

Chronic and acute inflammation is often attributed to oxidative/electrophilic stress in cells. Although many mechanisms and pathways exist to deal with this issue, one main pathway involving the regulation of the Keap1-NRF2 system is not fully understood<sup>1</sup>. On the path to creating targeted drugs towards oxidative/electrophilic stress, the sensing mechanisms must be understood. In this study, we created a computational model of the Keap1 homodimer starting from a crystal structure of a Keap1 mutant<sup>2</sup> (PDB 4CXI). The point mutations used to obtain a diffraction-quality crystal were corrected computationally. From this model, the local environment of a therapeutically important cysteine residue<sup>3</sup> (Cys151) was analyzed. Two histidines on the surface of this Cys151 local environment - His1289 and His154 - were examined for their potential protonation state in solution. The His129 was shown to switch conformations and move its imidazole ring  $\sim 5\text{\AA}$  compared to crystal structure data, indicating it is potentially not the native conformation. We did not observe any conformational changes in the His154 when protonated along with His129 indicating this may be present in the protein native state. Further studies are needed to investigate the protein on a larger scale as well as the effect of various electrophilic moieties binding to the cysteine thiol and their effect on the structure.

# Development of Gold Plasmonic Nanoarrays for Efficient SERS Sensing of Environmental Contaminants

**Najwan Albarghouthi (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best overall oral presentation in Analytical Chemistry

Division: Graduate Analytical

Public attention to the water contamination raises an urgent need to develop effective and reliable methods to detect the presence of any organic compound in water such as, atrazine. The current detection techniques for instance, liquid chromatography, mass spectroscopy, or colorimetric methods, which usually require sophisticated and time-consuming steps or sample preparation besides a well-trained operator. Herein, surface enhanced Raman is a powerful vibrational spectroscopy technique that allows for highly sensitive structural detection of compounds. Significant signal amplification is observed on roughened surface of metal nanostructure. However, developing a novel nanomaterial as cost effective, sensitive, and reproducible substrate for surface-enhanced Raman spectroscopy (SERS) applications remains a major challenge. Therefore, Gold nanorods (GNR) are a great candidate for SERS substrates, their importance rises from their LSPR excitation by light, which generates a strong signal due to their anisotropic shape. While great progress has been made in the synthesis of gold nanorods, relatively less success has been achieved towards ordering such structures into 2- and 3- dimensions in an effort to have a more uniform and robust sensing platform. This research work will explore two methods for the creation of multidimensional gold nanorod (GNR) arrays using both induced evaporation and Langmuir- Blodgettry.

# Development of a SERS-Based Rapid Vertical Flow Assay for Point-of-Care Diagnostics

**Kathleen Allen (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best undergraduate poster presentation in Analytical Chemistry

Division: Undergraduate Analytical

Point-of-care (POC) diagnostic testing platforms are a growing sector of the healthcare industry as they offer the advantages of rapid provision of results, ease to use, reduced cost, portability, and the ability to efficiently link patients to care. Chromatographic flow assay technology has been used for many POC testing, however; this technology has several disadvantages such as lack of sensitivity, along with limited capacity for multiplexing and quantitative analysis. Over the last several decades, surface enhanced Raman spectroscopy (SERS) has been used for the detection of biological analytes with high specificity and sensitivity. Coupling SERS with chromatographic flow assay technology will enable on-site acquisition, storage, and transmission of important healthcare metrics. In this work, SERS is coupled for the first time to a rapid vertical flow (RVF) immunotechnology for detection of anti-HCV $\alpha$ antibodies. High-quality and reproducible SERS spectra were obtained using gold nanoparticles (AuNPs) that have been modified with para-aminothiophenol (p-ATP). Many optimization studies such as variation of AuNPs size, p-ATP concentration and volume, and monoclonal antibody volume have been conducted to improve the SERS signal. It was observed that increasing the AuNPs size from 13 nm to 30 nm shows drastic enhancement in SERS signal. Also, increasing the volume of the AuNPs added to the RVF test cartridges enhanced the SERS signal and reduced spot-to-spot variation, resulting in increased reproducibility of the test results. A series of dilution studies were conducted that determined the detection limit is 1/2000 diluted antibody.

# Entropy and entanglement in quantum gravity: a delightful romp through mathematical physics

**Courtney Allen (University of New Brunswick-Fredericton)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Research Award, Mathematics and Statistics Oral Presentation, First Place

Quantum gravity is a physical theory that endeavours to provide a quantum mechanical description of gravity. The purpose of this project was to determine the gravitational field produced by the quantum state of a system, and how gravity aspects a property of these states known as entanglement. An entangled system is one whose particles are intertwined and cannot be thought of separately. The central question this project aimed to answer was: if a system begins in a product state—a system that we think of as non-entangled—does the system become entangled over time? The Newton-Schrodinger equation was used to model this situation. This equation couples the Schrodinger equation, which describes the time-evolution of a quantum system with an initial state  $\psi$ , with the Poisson equation, which determines the Newtonian potential  $\phi$  from the quantum state. Both the quantum state of the system and the gravitational field evolve over time under the Newton-Schrodinger equation. The Crank-Nicholson scheme, a method used to approximate derivatives in the Schrodinger equation, was used to produce numerical solutions to the Newton-Schrodinger equation. After plotting how the system evolves over time, the entanglement of the system can be determined by calculating its entropy. A product state has zero entropy, while an entangled state has some non-zero entropy. Thus, by calculating the entropy of the system, the entanglement can be determined.

## A Link Between Music Theory and Graph Theory

**Jordan Barrett (Dalhousie)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Communications Award

What makes a musical rhythm sound good? This fundamental question in music theory can be modeled by discrete methods in mathematics. Consider a hit song with an underlying beat. This beat normally cycles in groups of 16 short intervals, and so we could represent this beat as a directed cyclic graph  $C$  with 16 vertices, and with a set  $S$  in  $V(C)$  consisting of all the “hits” in the beat. In this talk we will explore 6 of the most popular rhythms in music history and determine which of these 6 dominates popular music. This will lead to a graph theoretic interpretation of the fundamental question: what makes a good rhythm good. We will see a connection between the “catchiness” of a rhythm and the “evenness” of points on the corresponding cycle. We will also ask the larger question of how to choose vertices on an arbitrary graph in the most “even” way possible, which will tie into the infamous facility location problem from computational geometry. No knowledge of music theory is needed, and only a basic core understanding of graph theory will be assumed.

# Development of a Methodology and Apparatus for In Situ Sampling of Polycyclic Aromatic Hydrocarbons in Natural Water Using Molecularly Imprinted Polymers

**Holly Victoria Barrett (Memorial University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of Science Atlantic Science Communication Award

Division: Undergraduate Analytical

Molecularly imprinted polymers (MIPs) are polymers formed in the presence of a template molecule. After polymerization, the removal of the template molecule leaves behind cavities in the polymer whose shape, size, and functionality are complimentary to the template, and hence these cavities can act as highly selective binding sites for specifically targeted analytes.<sup>1</sup> MIP formulations using a pseudo-template have been applied for the monitoring of a range of light polycyclic aromatic hydrocarbons (PAHs) in surface waters, as some PAHs are known environmental pollutants and suspected human carcinogens.<sup>2</sup> In the presentation, work involving the development of methodologies for the use of PAH MIPs for sampling of a group of six PAH compounds in large volumes of water, as well as the design and production of a sampling apparatus which can be used for in situ deployment in shallow rivers will be presented. This work will examine the advantages of a head space-gas chromatography-flame ionization detection (HS-GC-FID) method for the direct analysis of MIPs to establish a high-throughput methodology that allows for the direct detection and quantitation of PAHs in environmental waters with minimal sample preparation.

# Tricyclohexylphosphonium Ylidyl Substituents for a More Powerful Bispyridinylidene Organic Electron Donor

**Amar Kumar Bhardwaj (University of New Brunswick, Fredericton)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best overall poster presentation in Inorganic Chemistry

Division: Undergraduate Inorganic

Ground state organic electron donors and their use as reducing agents have gained more interest and investigation in recent times. More specifically however, it is the fine tunability of these organic reducing agents that is of interest. By modification of substituents on an organic electron donor scaffold such as a bispyridinylidene (BPY), different reduction potentials can be achieved. Previous work with the ylidic triphenyliminophosphorano ( $\text{Ph}_3\text{P}=\text{N}^-$ ,  $\sigma_{\text{p}^+} = -1.82$ ) and tricyclohexyliminophosphorano ( $\text{Cy}_3\text{P}=\text{N}^-$ ,  $\sigma_{\text{p}^+} = -2.21$ ) substituted BPY's has shown that the group attached to the phosphorous atom has a dramatic effect on the redox potential of the BPY and that the  $\text{Cy}_3\text{P}=\text{N}^-$  substituted compound yielded a stronger organic reducing agent ( $E_{1/2} = -1.51\text{V}$  vs SCE). More recently, Dyker and co-workers have found that a triphenylphosphonium ylidyl substituted BPY ( $\text{Ph}_3\text{P}=\text{CH}^-$ ,  $\sigma_{\text{p}^+} = -2.33$ ) exceeded the reduction potentials than the iminophosphorano substituted BPY's ( $E_{1/2} = -1.55\text{V}$  vs SCE). This has prompted the synthesis of the related tricyclohexylphosphonium ylidyl substituted BPY ( $\text{Cy}_3\text{P}=\text{CH}^-$ ), which is predicted to be the strongest disubstituted BPY organic electron donor to date. The synthesis of the tricyclohexylphosphonium ylidyl substituted BPY was attempted and the synthesis and characterization of its direct precursor will be described.

# Viral spread of Black Queen Cell Virus in managed and wild bees in Canada

**Emma Blanche (Acadia University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Poster Second Place

Native and managed pollinators are vital to Canada's agriculture and biodiversity; however, these species are currently facing population declines. One of the most prominent viruses affecting the western honey bee (*Apis mellifera*) is Black Queen Cell Virus (BQCV), which is fatal to developing honey bee queens. Previous genomic analyses have shown that interspecies transmission of pathogens is common between managed honey bees and wild bumblebees, while the BQCV genotypes tend to be most similar within the geographic site where they were collected. The objective of this study is to trace the spread of BQCV across *Apis* and native bee species within Canada to better understand viral transmission in pollinators. Bees were collected from sites across Ontario, Alberta, and Nova Scotia and were tested for BQCV. Viral RNA was extracted and PCR was used to amplify viral cDNA targeting the helicase gene. PCR products were sequenced using the Illumina MiSeq Next-Generation Sequencing platform and sequences were analyzed for genetic similarity. Phylogenetic analysis revealed sequences within Nova Scotia that clustered by geographic site, as well as some that clustered by bee genera. The viral sequences did not cluster neatly by province, though when compared to internationally collected sequences, they did cluster by country. These results suggest pathogen spillover between managed and native bee species across Canada, and that infected wild bees act as carriers for viral transmission even when appearing asymptomatic. Broader genomic analyses are needed to explore the transmission of BQCV across Canada, as the global data set remains limited.



## Targeted Soil Inoculation: Impact and Future Directions

**Kaitlyn Blatt-Janmaat (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best overall oral presentation in Biological and Medicinal Chemistry

Division: Undergraduate Biological and Medicinal

Food security is an issue worldwide. To provide enough food for our growing population, new agricultural practices must be investigated to ensure the long term viability and sustainability of the industry. In an attempt to increase the growth and yield of agricultural crops, several practices utilized by early farmers are being re-examined and improved. Two of these methods include biochar addition and soil inoculation. Biochar is a porous, pyrogenic material with a high carbon content formed from the slow pyrolysis of carbon heavy biomass. Introduction into the soil has yielded improvements in vegetative growth and nutrient retention. Soil inoculation is the practice of introducing beneficial microorganisms into the soil of the target host plant. When performed correctly, improvements in vegetative growth and plant immune response have been observed. A biochar-microbe composite has been produced and utilized as a means of targeted soil inoculation. Variable impacts on the vegetative growth, volatile production, and nitrogen content of plants has been observed with this technique. Implications for potential plant products, particularly wine, and future areas of research will be discussed.

# The Development of SpaceLaunch: A Faster App Launcher Developed in Unity

**Nathaniel Brewer (University of New Brunswick)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Research Award, Computer Science Oral Presentation, Second Place

In this presentation, I will discuss my experience developing SpaceLaunch -a smart phone application launcher that allows people to learn app locations more easily than conventional app launchers. Previous work has demonstrated that retrieval of digital items is faster when people are provided with an overview of an entire information space. SpaceLaunch provides an overview of all apps, allowing users to utilize spatial memory when learning the locations digital items. Current methods of organizing smart phone applications (e.g., folders and pages) don't allow users to take full advantage of spatial memory. SpaceLaunch is designed to utilize this important aspect of memory to decrease application location learning and retrieval time. To empirically test SpaceLaunch, we developed two other application launchers; one mimicking the folders organizational strategy and the other mimicking the pages strategy. In this talk I will focus on my experience using the Unity game engine to develop and test the SpaceLaunch prototype. I will outline our use of Unity in the context of Human-Computer Interaction (HCI) experimental prototype development, discussing issues that arose and how they were overcome. SpaceLaunch and its competitors were developed using the Unity game engine. Unity is a popular game engine with a large on-line community that supports 2D and 3D games. It also allows for deployment to over 25 platforms (e.g., Android, iOS, HoloLens, PS4, etc.). e comprehensive tools (including IDE, community, Room C# support, and build tools) associated with Unity provide opportunities for HCI researchers to rapidly develop, deploy and test experimental HCI systems.

# The performance of biocide and non-biocide coatings to prevent biofouling by invasive and non-native species in Newfoundland

**Ashley Bungay (Memorial University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Graduate Research Award, First Place

Biofouling, the unwanted growth of aquatic organisms can characterize invasion hotspots and vectors for spread of non-native species with implications for industries (e.g. aquaculture). In shellfish aquaculture, fouling by invasive tunicates directly on the species can reduce oxygen and food acquisition, leading to slower growth. For example, biofouling by vase tunicate (*Ciona intestinalis*) in Prince Edward Island, Canada causes significant increases in time and labour to remove and process product. Traditionally, antifouling coatings are used in aquaculture industry to limit fouling, not the spread of non-indigenous species. Self-polishing copolymer coatings contain biocides; others, foul-release coatings, rely of physical properties of the coatings (smoothness. Concerns of toxicity of biocides (e.g. copper) have led to development of new coatings. In our study, deployed wood settlement panels tested eleven coatings (and two controls) at four sites that characterize Newfoundland fouling communities and three invasive tunicate species (*C. intestinalis*, *Botrylloides violaceus*, and *Botryllus schlosseri*). Four coatings contained cuprous biocides, two used zinc biocides, one used zinc and Ecomea™ as biocides, two were foulrelease coatings (non-biocide), and two were non-antifouling marine paints. We photographed panels monthly (May to December 2016) to determine changes in percent coverage of biofouling communities. Preliminary results suggest biocide coatings prevent growth of fouling organisms most effectively (as low as 0% coverage), while panels with non-antifouling marine paints exhibited up to 100% coverage, including invasive tunicates. Although, the most effective coatings contained biocides, one foul-release coating showed limited biofouling and may present a non-biocide alternative for use in the aquaculture industry.

## Nest density of orange-belted bumble bees

**Brock Burgess (Acadia University)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

K.C. Irving Environmental Science Centre Award

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Poster Third Place

Pollination services are critical for global biodiversity and agriculture. Global pollinator declines have been well documented, putting the delivery of ecological services at risk. Despite global importance of wild pollinators such as bumble bees (*Bombus* spp.), little research has investigated their nesting preferences. As a ubiquitous species in Atlantic Canada, orange-belted bumble bees (hereafter, bumble bees), *B. ternarius*, provide important pollination services, making them an ideal candidate for this study. Objectives of this study were (1) to use microsatellites to estimate sibling relationships (and thus, indirectly, nest density) in worker bumble bees (*B. ternarius*) in agricultural systems, and (2) to evaluate the relationships between land cover and nest density. Six microsatellites were amplified from bumble bee workers collected from three different locations with different landscape configurations. Although the number of workers varied greatly among sites, the ratios of nests to workers were similar (0.79, 0.83, 0.85). More bees nested in evenly distributed, heterogeneous landscapes with agricultural components. This confirms that crops are valuable foraging resources for this bumble bee, and suggests that a diversity of landscape features is a driver of bumble bee nesting. Ultimately, nesting preferences of bumble bees need to be further explored, because this study was constrained to only three study sites.

## A Strong Electron Donor via the Superior $\pi$ -Electron Donating Ability of a Triphenylphosphonium Ylidyl Group

**Morgan Burgoyne (University of New Brunswick, Fredericton)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of E. Gordon Young Award for Best Graduate Pedagogical Presentation

Division: Graduate Inorganic

The  $\pi$ -electron donor strength of a triphenylphosphonium ylidyl group ( $\text{Ph}_3\text{P}=\text{CH}^-$ ) was explored through its substitution onto a bispyridinylidene (BPY) scaffold. Electrochemical studies revealed that the triphenylphosphonium ylidyl-substituted BPY is the most reducing di-substituted derivative reported to date ( $E_{1/2} = -1.55$  V vs. SCE), which exceeds the reduction potentials of the iminophosphorano counterparts. The utility of this new organic reductant will be exhibited through its use in metal-free reductions targeting new organic substrates. Additionally, by using a previously established correlation, the redox potential of the substituted BPYs allowed for the determination of a Hammett constant for the  $\text{Ph}_3\text{P}=\text{CH}^-$  group ( $\sigma_{\text{p}^+} = -2.33$ ), showing it to be the most donating neutral substituent currently known. The information about the donor ability of the methylenephosphorano groups from this study should be broadly applicable and will allow for new and more reducing organic electron donors to be targeted.

## Building Entangled Photon Triplet Source by Cascaded Spontaneous Parametric Downconversion

**Yannick Castonguay-Page (Université de Moncton)**

Presented at the 37<sup>th</sup> Atlantic Undergraduate Physics & Astronomy Conference, February 2-4, 2018

The Tindall/Steinitz Award in Research, First Place Tie

Polarization-entangled photon triplets are an important resource for several quantum information applications, namely for quantum cryptography. Such photon triplets can be produced through cascaded spontaneous parametric downconversion, by combining two sources of polarization-entangled photon pairs. Here, we present our recent work towards the creation of a phase-stable source of polarization-entangled photon triplets. Using a periodically poled potassium titanyl phosphate (PPKTP) crystal, we produce the first pair of polarization-entangled photons through spontaneous parametric downconversion (SPDC) within a Sagnac interferometer. We then characterize this first source using quantum tomography, confirming the quality of the entanglement. Going forward, this first SPDC process will be combined with a second SPDC source composed of another Sagnac interferometer but with a periodically poled lithium niobate (PPLN) waveguide to produce polarization-entangled photon triplets.

## The bountiful coprolites of the Joggins Formation

**Max Chipman (Acadia University)**

Presented at the 67th Atlantic Universities Geological Conference, October 26-28, 2018

Canadian Society of Petroleum Geologists (CSPG) Award

The fossil cliffs at Joggins (Nova Scotia) hold a wealth of fossils, both terrestrial and aquatic, from the Late Carboniferous Period. Fossils from the aquatic realm have historically been understudied and the ecosystem they represent is poorly understood. This research broadens our understanding of the aquatic ecosystem, specifically the food web, by examining fish coprolites that are abundant in the limestones of the Joggins Formation. Coprolites preserve undigested material that give us a window into the diets of these fish and a better idea of species interactions within the ecosystem. The coprolites have been studied in thin section and hand sample, as well as cathodoluminescence and computed tomography to determine the contents. We found that specimens could be divided into six categories based on size and shape: cigar/cylindrical shaped; cone shaped; small/equant; spiral; irregular; and massive (samples greater than 5 cm in length). The small coprolites are the most abundant and the massive coprolites are the rarest. They range in size from 10 cm and are 2-3 centimetres on average. The mineralogy of the coprolites is high calcium phosphate, similar to the composition of bone. This suggests that the fish producing these coprolites were carnivorous and that there is a lack of herbivores present, supporting Carpenter et al.'s (2015) faunal study findings. Bone fragments have been found in almost all samples, however specific species identification has thus far been impossible. This research provides both a foundation for further studies on coprolites and similar fossils and a deeper understanding of aquatic ecosystems as fish diversified further into fresh water in the Palaeozoic.

## The relationship between anal fin size and behavioural traits of male Japanese medaka, and their importance in reproductive success across varying social settings

**Victoria Cluney (Saint Mary's University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Poster First Place

Sexual selection leads to the development of secondary sex traits and mating behaviours. Morphological and behavioural traits serve to increase reproductive success among individuals, however, under varying sexual selection types and intensities the relative importance of particular morphologies and behaviour will vary. This study examines the relationship between morphology and behaviour of male Japanese medaka (*Oryzias latipes*) and their importance in reproductive success across varying social settings. During mating, males perform a variety of behaviours including aggression and courtship. In addition, males use their anal fin to grasp the female during mating, and reduction in anal fin size is associated with lowered fertilization success. In this species, there is natural variation in sex ratio during mating across latitude, and this variation is associated with differences in reproductive behaviour and anal fin size. By subjecting the male medakas to four different operational sex ratios (defined as the ratio of fertilizable females and sexually mature males), we were able to manipulate sexual selection pressure intensity in the laboratory. Anal fin size, aggression and courtship behaviours were quantified for all treatments. Ongoing analysis suggests that as the operational sex ratio becomes extremely male biased, male aggression increases in frequency, and courtship behaviour decreases in frequency. These results indicate that the social environment influences the behavioural tactics used to obtain mates, and that males are plastic in their response to different intensities of sexual selection.



## Photocatalytic Applications of AuNP/Perovskite Hybrids in C-C Bond Formation

**Bry W. Crabbe (St. Francis Xavier University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best graduate oral presentation in Materials Chemistry

Division: Graduate Materials

Heterogeneous catalysis has garnered considerable attention over the past decade as a means of implementing more sustainable chemical routes through the use of environmentally benign energy sources (light) and minimizing undesirable toxic chemical waste and byproducts. Perovskite potassium niobium oxides are an underdeveloped class of semiconductor materials, with properties similar to TiO<sub>2</sub>, that allow for ease of removal from reaction solutions due to its larger particle size. Nanoparticle functionalization (Au, Pd) of the potassium niobium oxide surface will enable greater charge separation on light activated semiconductor surface, allowing for more effective exploitation of its photoredox states. In the following contribution, the light-driven reactivity of these solids will be examined for applications in the photocatalytic C-C homocoupling reactions of iodobenzene and phenylboronic acid, respectively. Preliminary results illustrate proficient and selective coupling of the substrate molecules to form the coupled biphenyl product. Surprisingly, the monometallic, AuNP-potassium niobium oxide composites produce high product yield in iodobenzene coupling while PdNP-potassium niobium oxide hybrids perform best in the corresponding phenylboronic acid reaction. The effects of metal nanoparticle loading, metal nanoparticle properties, light source, reaction time, reaction components and recyclability of photocatalyst will be examined and directly correlated to the efficiency of light induced carbon-carbon bond formation.

## Microplastic export from wastewater treatment plants in New Brunswick rivers

**Taylor Crosby (Mount Allison University)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

Science Atlantic Undergraduate Research Award, Oral Presentation, First Place

Microplastics are a ubiquitous contaminant found worldwide in terrestrial, freshwater, and marine environments. These contaminants are defined as any plastic smaller than 5mm. They cause concern once they enter the food web. There are high abundances known to exist in the ocean but relatively few studies focus on freshwater microplastic contamination. This study focuses on 10 sites in 7 different rivers across South-Eastern New Brunswick receiving varying amounts of waste water effluent. We investigated whether waste water treatment facilities are a point source for microplastics and if they are being transported further downstream. Using standard methods, water column samples and sediment samples were collected upstream and downstream from treatment facility effluent discharge points, which are predicted to be a source of this contaminant. Microplastics were present in every sample that was collected. In comparing samples collected upstream and downstream we determined based on our observations that more plastics were found proportionally downstream of waste water treatment outfalls. Our findings aid in the understanding of the origin of microplastics in the aquatic environment to mitigate for their impact on ecosystem health.

## An Exploration of 2D-LC-SERS: A Novel Detection Modality for Multidimensional Chromatography

**Melanie Davidson (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best overall oral presentation in Analytical Chemistry

Division: Graduate Analytical

Multidimensional liquid chromatography (2D-LC) provides substantially better resolving and separating power than conventional high pressure liquid chromatography (HPLC), and over the past decade has been applied in many different fields of chemistry.<sup>1</sup> The current gold standard for detection modalities in conjunction with LC is mass spectrometry (MS). However, this technique is data heavy, it isn't portable, and the instrumentation can be very expensive.<sup>2</sup> This research will couple the emerging technique of 2D-LC with the sensing power of surface-enhanced Raman spectroscopy (SERS) as a new detection modality. In order to exploit this detection technique, a SERS substrate must be optimized. Many different 3D-substrates were investigated for their use in phenolic acid detection. It was found that generic laboratory filter paper covered in pyridine functionalized silver nanoparticles gave the most promising results. These substrates will be used for further investigation and coupling of SERS to 2D- LC.

# Spatiotemporal assessment of metal concentrations of pre-effluent estuarine sediments in a freshwater kraft pulp mill tailings pond using paleolimnological methods

**Kirklyn Davidson (Acadia University)**

Presented at the 67th Atlantic Universities Geological Conference, October 26-28, 2018

Atlantic Geoscience Society (AGS) Environmental Geoscience Award

Paleolimnological research at a former estuary in Pictou County, NS that has been contaminated by effluent from a kraft pulp mill and other inputs over the past 50 years has focussed on understanding the spatiotemporal distribution of metals within pre- and post-disturbance sediments. The site was dammed in 1967, effectively converting it into a shallow freshwater lake (140 ha, 4 m max. depth). The lake bottom sediments within Boat Harbour reflect both estuarine and fresh water environments, and can be broadly characterised as grey marine clay (~ 50% water content) which is overlain by black, organic-rich sediment (~ 90% water content). The contact between these two units is sharp and is present through the basin. To inform post remediation management decisions the marine sediment was analysed for the spatiotemporal distribution of As, Cd, Cr, Cu, Pb, Ti, Zn, Mo, and Ni, which were identified as uniquely representative of impact at the site. The samples were collected using a gravity corer, were analysed for metal concentrations using pXRF and ICPMS techniques and distribution was modelled using QGIS. Preliminary results indicate that As, Cr, Cu Zn and Pb concentrations at reference sites meet or exceed ISQG's. Metal loads within the grey marine clay at the impacted site are similar to or higher than those at the reference sites. Metals in the marine sediment at the impacted site and the reference sites show little stratigraphic variability, indicating that overprinting of contaminants from the overlying organic sediment at the impacted site is not likely. Spatial distribution maps of metals are being completed; preliminary results indicate that there is substantial variability in metal concentrations spatially. These data must be taken into consideration in both the remediation and compliance stages of environmental assessment at the site.

## Temporal stability of genomic differentiation between spawning season components in Atlantic herring (*Clupea harengus*)

**Hillary Dort (Acadia University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Miramichi Striper Cup

Striped Bass (*Morone saxatilis*) are native to the Atlantic coast of North America and are recognized for their ecological, economic and cultural significance. Anthropogenic effects such as handling and angling, can negatively affect the health of striped bass populations. These effects can cause physiological and behavioral changes which are noticeable at individual, population, and ecosystem levels. Proteomic techniques were used to isolate, identify and characterize novel protein biomarkers in Striped Bass epidermal mucus and to investigate changes in protein profiles as a result of angling. Our methods included isolating proteins of interest in the epidermal mucus, as well as quantifying and exploring how specific protein biomarkers may play a role in determining fish health. Data obtained from 1D polyacrylamide gel electrophoresis and mass spectrometry analyses has identified putative protein biomarkers in Striped Bass epidermal mucus. Changes in protein profiles were correlated with known stress indicators and previously identified biomarkers. We have also characterized proteolytic activity in the mucus using zymography, which provides information on the class of proteases activated during stress-related events. By identifying biomarkers of stress in Striped Bass epidermal mucus we have defined a novel method for measuring stress in these fish which may contribute to a better understanding of the effects of angling stress on fish in general. We anticipate by recognizing the potential pitfalls in the handling and treatment of Striped Bass that this study may improve conservation decisions and regulations that will help to maintain healthy populations of Striped Bass, while still allowing recreational fishing.

# Nanocomposites as Catalysts for Biomass Transformation in High Value Added Products

**Andrew C. Duffy (St. Francis Xavier University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best undergraduate oral presentation in Organic Chemistry

Division: Undergraduate Organic

The development of green processes to transform cellulose and lignin, the most abundant renewable biomaterials on Earth, is of the utmost importance for sustainability given their biocompatibility and potential as alternative fuels. Heterogeneous semiconductor photocatalysis is also central to this process. The structure, size and porosity of the solids can be manipulated to greatly improve catalytic activity. Moreover, visible light, ideally sunlight, can be exploited as a green energy source and converted into chemical energy in an environmentally benign manner. This contribution will discuss the design of multifunctional nanoparticle/Nb<sub>2</sub>O<sub>5</sub> composites, exploiting the acidic, photocatalytic and photothermal capabilities of these heterogeneous materials to compliment the molecular characteristics of biomass. In particular, the photocatalytic aspect of these materials affords an opportunity to perform both oxidative and reductive processes after adsorption of one photon of light – increasing the effectiveness of these light-activated systems. Biomass conversion catalysts must be stable under hydrothermal conditions, i.e., moderate temperatures and high water concentration, unfavourable in petroleum processing. The dual acidic/photocatalytic activities of niobium oxide materials may afford the ability to catalyze different reactions using the same catalytic bed in an effort to reduce the complexity of biomass transformations. Nanoparticles (Au and Ag) will be used to extend the response of the material into the visible region of the electromagnetic spectrum, due to their unique absorption characteristics. The catalytic capacity of several nanocomposites will be discussed, as well as the potential reusability of these materials, given the focus on renewable resources and sustainable green chemistry initiatives.

# Examining the Role of the Parietal Cortex in Motor Imagery

**Mariam El-Serafi (Dalhousie University)**

Presented at the 42nd Science Atlantic Psychology Undergraduate Conference, May 8-9, 2018

Karen Nicholson Award in Neuropsychology

Motor Imagery (MI) is the mental performance of a motor task. It can be categorized into explicit MI, where performance is intentional and conscious, and implicit MI, where performance is induced or unconscious (Jeannerod and Frak, 1999). Motor imagery particularly relies on the inferior parietal lobe (IPL), commonly damaged post-stroke (Héту et al., 2013). Damage to parietal regions or inhibition to the left IPL diminishes the ability to perform explicit MI (Kraeutner et al., 2016). However, it is unknown whether the same inhibition to the left IPL can diminish one's ability to perform implicit MI. In this study, a 'virtual lesion' was induced via non-invasive brain stimulation using repetitive transcranial magnetic stimulation (rTMS). Seventeen participants received either inhibitory stimulation to the IPL or sham stimulation. Participants followed with performing two MI tasks measuring explicit MI, the Movement Imagery Questionnaire (MIQ), and implicit MI, the Hand Laterality Judgement Task (HLJT). Explicit MI ability was assessed using the MIQ score and mental chronometry, and implicit MI ability was assessed using the HLJT reaction time (RT) and accuracy. We hypothesized that the left IPL will be similarly involved in both types of imagery, specifically, it was expected that there will be decrements in performance on both MI tasks following active rTMS. We did not find significant effects of IPL inhibition on explicit or implicit MI ability. Our findings on explicit MI contradict previous research while the findings on implicit MI suggest that inhibitory stimulation to the IPL does not affect implicit MI ability.

## Macromolecular dynamics of *Thalassiosira weissflogii* under steady-state and non steady-state phosphorus stress

**Sally Faulkner (Mount Allison University)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

Science Atlantic Undergraduate Research Award, Oral Presentation, Second Place

Phosphorus (P) is a key limiting nutrient in the global ocean. There is relatively little data on the links between P availability and the biochemical and macromolecular composition of marine phytoplankton. To better understand P allocation in phytoplankton across a gradient of P stress, we investigated P content and major macromolecular composition in the common marine diatom *Thalassiosira weissflogii* under three P stress regimes; steady-state P-replete conditions (P5.0, 5.0  $\mu\text{M}$  phosphate), and two limiting P concentrations; 0.5  $\mu\text{M}$  and 0.25  $\mu\text{M}$  phosphate. Additionally, P5.0 and P-limiting (P0.25, 0.25  $\mu\text{M}$  phosphate) cultures were allowed to progress into non-steady state P starvation and sampled from exponential to stationary growth phase. Under P5.0 conditions, cellular phosphorus ( $P_c$ ) declined by 96% and total cellular protein declined by 40%. Under P0.25 conditions,  $P_c$  declined by 63% and total cellular protein declined by 8%. Cellular phospholipid P and RNA P content account for an increasing proportion of  $P_c$  present as cells progress to starvation, and comprise an overall higher proportion of  $P_c$  under P0.25 conditions. Based on these results we infer that diatom cells store more P when exposed to high phosphorus conditions. Further work is required to characterize P storage molecules.



## The Uptake of Sterols by $\beta$ -Cyclodextrin MOFs

**Livia Ferland (University of New Brunswick, Fredericton)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC third best overall poster presentation in Inorganic Chemistry

Division: Undergraduate Inorganic

The aim of this project is to create a metal organic framework that may act as a sponge for cholesterol. We have tried to design it to be stable enough to survive in the human body without deteriorating. It was found that a metal organic framework composed of  $\beta$ -cyclodextrin (CD) and potassium can uptake sterols within its pores due to their channel-like structures. Using these sterol-soaked crystals, the MOFs have been analyzed to visually show the channels within the structure as well as interpreted to find the abundance and rate of sterol diffusing out of the pores. Additionally, performing a metal ion exchange with heavier metals (Europium and Terbium) was done to make the crystal structure more stable as well as less soluble in water. They were then analyzed to see if the composition was as expected as well as to find any impurities within the structures.

## The ecology and effects of the bark beetle species, *Dryocoetes krivolutzkajae*, on roseroot populations in Newfoundland, Canada

**Allison Ford (Memorial University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Botany Award, Oral Presentation

Plant pathogens and insect pests can have detrimental effects on plant populations by impacting growth, reproduction, and survival. *Rhodiola rosea* L. (Crassulaceae), commonly known as roseroot, is a culturally-important medicinal plant that grows in coastal ecosystems across the Northern Hemisphere. Since roseroot is endangered in parts of its range, studying the effects of pathogens and pests on this species is important for its conservation. *Dryocoetes krivolutzkajae* Mandelshtam (Coleoptera: Circulionidae: Scolytinae) is a bark beetle that infests the rhizomes of roseroot, forming galleries and causing belowground plant tissue loss. Prior to this study, *D. krivolutzkajae* had been found in roseroot in Labrador, but was unknown to the island of Newfoundland. The objective of this study was to determine the presence of *D. krivolutzkajae* on the island of Newfoundland, to gain insight into the ecology of this insect herbivore, and understand its effect on the growth and survival of roseroot. Sampling plants from coastal areas of Newfoundland, I tested whether *D. krivolutzkajae* exhibited an affinity for roseroot plants of different biomass, number of shoots, and sex, as well as plants growing in different sites, distances from the shore, and substrates. Substrate types consisted of organic soil, bedrock, soil over bedrock, limestone gravel, beach soil, and gravel. *D. krivolutzkajae* was found to be present in Newfoundland, and no apparent affinities to substrate, number of shoots, distance to shore, or plant sex were observed. Presence of beetle galleries and higher amounts of rhizome damage were associated with roseroot plants having significantly larger biomass.

## Undergraduate-Led Computer Science K-12 Outreach

**Anna Luise Frankfurt (University of Prince Edward Island)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Research Award, Computer Science Oral Presentation, First Place

This report considers the first offering of an undergraduate-led computer science outreach program. This program focused on junior high students (grades 7-9), utilizing a week-long after-school boot camp. The undergraduate mentors organized, planned, and executed the entire program wherein the students had an introduction to computational thinking, computer programming, and a diverse group of undergraduate computer science students with a broad range of interests. The program required minimal involvement from the university faculty and staff and was almost entirely run by the undergraduate computer science mentors recruited from the university student body. The goals of the program were to give an opportunity for junior high students to learn about computer science and to share with them the image of a computer scientist, where otherwise these students may have never been exposed. The program was beneficial to the undergraduate students by offering an opportunity to showcase skills such as but not limited to curriculum planning, teamwork, communication, and teaching. This program was successful enough that it is now a part of ongoing university engagement planning. This report presents experience running the program as well as survey results from our participants.

# Cyclometalated Ru(II) Dyads as Highly Selective Photosensitizers in Photodynamic Therapy

**Anderson M. Fuller (Acadia University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC Physical, Theoretical and Computational Chemistry

Division: Undergraduate Physical, Theoretical, and Computational

Photodynamic therapy (PDT) is a form of cancer treatment that utilizes nontoxic, light-responsive compounds that can be activated with photons to destroy cancer cells with spatiotemporal selectivity. Historically, porphyrin-based compounds have been used as photosensitizers and function by producing cytotoxic singlet oxygen ( $^1O_2$ ) from triplet  $^3$  excited states. We have invested efforts into developing coordination complexes as alternatives to these organic systems to access additional excited states that employ oxygen-independent mechanisms for photocytotoxicity. In this study, we developed Ru polyridyl complexes of the type  $[Ru(dmb)_2(LL)]^+$  that incorporate C<sup>N</sup> ligands with differing number of rings in the of -oligothienyl functional ligand. These Ru(II) C<sup>N</sup> complexes are both more photochemically stable and have red-shifted absorption profiles. These are attractive properties that triggered an investigation into the less studied domain of C<sup>N</sup> complexes over their more popular counterpart, Ru(II) N<sup>N</sup> complexes. The investigation on these four complexes demonstrated that as we increase the length of the -expansive functional ligand, we get increased access to 3IL states, an increased phototherapeutic index (PI) and we found that this group of metal complexes could serve as highly selective chemotherapeutic agents and others are extremely potent photocytotoxic agents.

## Low Surface Area Alloy/GIC Composites for Lithium Ion Battery Anodes

**Shayne Gracious (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best undergraduate oral presentation in Materials Chemistry

Division: Undergraduate Materials

Composite materials for lithium ion battery anodes were synthesized by combining various powders with poly(acrylic) acid (PAA). These powders were based on combinations of a Si-Fe alloy and an aluminosilicate glass. It was found that the composite materials showed an increase of particle size relative to that of the initial Si-Fe alloy while retaining the Si-Fe crystalline phases. Furthermore, the introduction of aluminosilicate glass improved the water stability of the composite materials. The use of high shear mixing as a method of electrode slurry formation was also explored. This yielded electrodes that had reduced polarization, but formed crystalline  $\text{Li}_{15}\text{Si}_4$  phase throughout cycling. The use of the composite materials in these electrodes suppressed the formation of this phase. Despite the formation of this phase in some of these electrodes, they showed good cell performance.

# A High Resolution Record of Sediment Deposition in the Gulf of Aqaba during the last ~1000 years

**Ariel Greenblat (Dalhousie University)**

Presented at the 67th Atlantic Universities Geological Conference, October 26-28, 2018

Science Atlantic Best Paper Award

The Gulf of Aqaba is a narrow and deep basin at the northeastern tip of the Red Sea. Sedimentation is dominated by biogenic and eolian material, as well as by material delivered by the Wadi Mubarak. Here we present paleoenvironmental proxy records from a 108 cm gravity core, recovered at 720 m water depth at the northern end of the Gulf. These records are compared to sediment flux directly sampled by co-located sediment traps deployed since 2014, which show that sedimentation is dominated by sporadic, short-lived flux events on the order of days. An event deposit in the sediment core at 96- 87 cm, with coarse sediment at the bottom and a fining upward sequence is tentatively, and in analogy to previous studies, ascribed to a turbidite triggered by the historical earthquake at 1068 AD. This age assignment would imply overall sedimentation rates on the order of 1 mm/yr at our sampling site, in general agreement with bulk flux estimates from the sediment traps as well as previously published sediment core records from the Gulf of Aqaba. Records of basic sediment geochemistry, foraminiferal abundances, and nitrogen isotopes will be discussed in the context of regional climate, hydrographic variability, and nitrogen cycling during the last 1,000 years.

# The impact of carbon surface oxides on self-discharge in acidic-aqueous-electrolyte electrochemical capacitor electrodes

**Alexander Hare (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC Physical, Theoretical and Computational Chemistry

Division: Undergraduate Physical, Theoretical, and Computational

It is well known that when oxidized, carbon electrochemical capacitor (EC) electrodes form a variety of carbon oxides, such as quinones, lactones, ethers, and carboxylic acids. While some improve capacitance (e.g. pseudocapacitive quinone groups), the impacts that these surface functionalities have on carbon self-discharge is not understood. This project studies the impacts of oxygen surface functionalities on the self-discharge of four carbon powders: Vulcan XC72, pristine birch biochar, HNO<sub>3</sub>-oxidized biochar, and KOH-oxidized biochar. It is extremely important to develop an understanding of self-discharge mechanisms for ECs because it allows for the development of preventative measures that stop self-discharge from occurring, enabling the development of more efficient and reliable charge storage devices. To study the effect of oxidation on self-discharge, cyclic voltammetry (CV) and open-circuit potential self-discharge measurements were run in 1 M aqueous H<sub>2</sub>SO<sub>4</sub> electrolyte. X-ray photoelectron spectroscopy (XPS), thermally programmed desorption (TPD), and CV were performed in order to determine degree and type of oxidation. Comparison is made between the self-discharge of each carbon material before and after oxidation through repeated CV cycling, as well as between the first and last charge/self-discharge cycles. It has been shown that self-discharge decreases for all carbons as self-discharge cycling repeats. Fully oxidizing Vulcan is shown to have a minor impact on its self-discharge. Fully oxidized KOH-oxidized biochar showed less self-discharge compared to its as-received state. Pristine birch biochar was found to be a poor EC, and self-discharge for HNO<sub>3</sub>-oxidized biochar showed little change, likely because its surface was already fully oxidized.

## Examining the Large-Amplitude Proton-Tunnelling Behaviour in Malonaldehyde

**Ryan Harvey (University of New Brunswick-Fredericton)**

Presented at the 37<sup>th</sup> Atlantic Undergraduate Physics & Astronomy Conference, February 2-4, 2018

Science Atlantic Science Communication Award

Imagine this: you roll a ball up a hill, but it wasn't fast enough to go over, so it just rolls back down. Now try again with the same initial speed, but this time it pops out on the other side of the hill. This is a rough analogy to quantum tunnelling. Since quantum mechanics is all about probabilities rather than deterministic measurements, a particle that doesn't have enough energy to overcome some potential energy barrier may still be found on the other side. The organic molecule malonaldehyde is a good example of this. In malonaldehyde, one hydrogen atom has two equivalent equilibrium positions separated by an energy barrier, and it can tunnel through this barrier. Thus, malonaldehyde is a sort of natural laboratory for studying the tunnelling effect, because while the proton is more or less a quantum blur, the rest of the nuclei in the molecule move relatively little. Other than motion due to rotation of the molecule as a whole, these other nuclei only have small amplitude vibrational motions, much less dramatic than the tunneling motion. Using data from the Canadian Light Source (CLS) synchrotron in Saskatoon, we are studying the effects of tunnelling on the spectrum of the molecule, as well as the effect of replacing the tunnelling proton with a deuteron. We are also developing a model to describe the way the molecule's structure changes while the tunnelling occurs.



## Response of intertidal communities on a tidal gradient to high and low suspended sediment concentrations

**Eileen Haskett (Acadia University)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

Science Atlantic Graduate Research Award, Oral Presentation, Second Place

Suspended sediment is an important, yet overlooked, factor in the survivorship of intertidal invertebrates that rely on its availability for food and shelter. In this study we investigated how the taxonomic and functional diversity of tidal flat invertebrates is affected by high and low concentrations of suspended sediment. Cores were collected from low-, mid-, and high-intertidal zones in the Minas Basin and placed in tidal mesocosms with either low (10 – 30 mg/L-1 ) or high (100-400 mg/L-1 ) suspended sediment concentrations for up to four weeks. Invertebrates were sorted and identified to determine changes in diversity. Sediment characteristics (chlorophyll concentration, organic content, sediment composition) were also analyzed. Species from the low-intertidal zone were negatively impacted by low suspended sediment concentrations; for example, key species *Clymenella torquata* and *Spiophanes bombyx* dropped in abundance, and deposit-feeding, herbivorous, and scavenging functional groups also decreased. Species from mid- and high-intertidal zones responded positively to being placed in the mesocosm, with key species (*Chaetozone setosa*, *Pygospio elegans*, and *Streblospio benedicti*) and most functional groups maintaining or increasing in abundance at both sediment levels. Sediment characteristics from all intertidal zones were unaffected by treatment. The sensitivity of the low-intertidal zone to a decrease in suspended sediment concentration raises the question of how it will respond to anthropogenic factors (i.e., tidal turbine farm implementation) that alter tidal flow and associated suspended sediment, potentially impacting the predators, including migratory shorebirds and endangered Atlantic sturgeon that rely on the low-intertidal invertebrates for food.

## Benchtop Borenum Catalysis

**Blake Huchenski (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best graduate oral presentation in Organic Chemistry

Borenum catalysis has undergone a rapid development in recent years, providing highly active catalysts in hydrogenation and hydrosilylation chemistry. Small molecules such as DABCO and lutidine have been highlighted in recent publications to stabilize borenum ions<sup>1,2</sup>. This chemistry has been applied in catalytic reactions using common boranes as reagents. However, these catalysts are often highly moisture sensitive and require dry conditions for use. Catalysts are often prepared before use, as the reagents used for preparation of borenum cations are themselves often active catalytically. This work provides an account of a new moisture tolerant system which provides access to borenum chemistry on the benchtop in common solvents without the use of solvent drying or purification. This system can also be applied to hydrogenation and hydrosilylation chemistry with the aid of carbene borane complexes<sup>3</sup>.

# Molybdenum Carbide Nanostructures for Efficient Electrochemical Hydrogen Evolution

**Govinda Humagain (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best undergraduate poster presentation in Materials Chemistry

Hydrogen is the next generation energy source to produce electricity from its stored chemical energy. Sustainable and affordable production of hydrogen is extremely important for extensive commercialization of fuel cells. However, efficiently carrying out the hydrogen evolution reaction (HER) in acidic solution without Pt remains challenging. In the last few years, there has been a concerted effort to develop cheap, active, and stable HER catalysts. Transition metal carbides (TMC) have received considerable attention as alternative electrocatalysts and supporting materials due to either a decrease in the amount of Pt required or in some cases, complete removal of the precious metal. In this study, we show formation of Mo<sub>2</sub>C electrocatalysts derived from biochar that shows HER performance similar to Pt metal at 10 mA/cm<sup>2</sup> but better performance at 100 mA/cm<sup>2</sup>. The catalysts also showed long-term chemical and mechanical stability. The synthesis of this catalyst is scalable and cheaper than the methods reported previously.

## Spatio-temporal mapping and analysis of the Atlantic Halibut (*Hippoglossus hippoglossus*)

**Isabelle Hurley (Dalhousie University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Second Place

Science Communication Award

Fisheries bycatch in Atlantic Canada Atlantic Halibut (*Hippoglossus hippoglossus*) is currently the most valuable commercial groundfish species per unit weight in Atlantic Canada. The fishery is performed by longliners using bottom gear with approximately 1000 hooks per fishing set, which are known to accidentally catch substantial amounts of non-targeted species (bycatch). Since 1998, Fisheries and Oceans Canada and the Halibut fishing industry have performed annual joint surveys on the Scotian Shelf and Southern Grand Banks to monitor both the Halibut catch and bycatch. This survey data was used to examine the spatial and temporal bycatch trends from 1998 to 2016. Maps were produced to observe spatial patterns and linear regressions were used to determine temporal trends in these metrics in different fishing areas. Over 95 species were identified in the bycatch of the Atlantic Halibut longline fishery, including: marine mammals, seabirds, benthic invertebrates, finfish, sharks and skates. Some of these species are listed under the Species at Risk Act (SARA), specifically the threatened Northern Wolffish (*Anarhichas denticulatus*) and Spotted Wolffish (*Anarhichas minor*), and 15 species are listed by the Committee on the Status of Endangered Wildlife in Canada (COSEWIC). From 1998 to 2016, Spiny Dogfish were caught at nearly a 3-fold higher frequency than Atlantic Halibut. The produced maps indicate highest bycatch amount and species richness on the Southern Scotian Shelf and the Southern Grand Banks. The revealed temporal trends and spatial patterns of bycatch help to understand the ecosystem impact of the Atlantic Halibut fishery and can inform fishery management and marine conservation.

## Regioselectivity Studies of Anionic 5-exo/6-endo-dig Cyclization toward Pyrrolone and Pyridinone

**Genesis Infante (University of New Brunswick, Fredericton)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best graduate oral presentation in Organic Chemistry

Thieno-, furano-, and pyrrolo-alkynylamides were synthesized and cyclized into pyrrolone (5-exo-dig) and pyridinone (6-endo-dig) products. The competing cyclization pathways were explored experimentally and computationally, providing access to these new class of heterocyclic molecules currently unavailable by other methods.<sup>1</sup> The 5-exo-dig cyclization pathway is usually disfavoured in heterocyclic systems, and 6-endo products are often both the kinetic and thermodynamic products. Shifting the favourability toward the 5-exo-dig can be achieved by changing factors such as heteroatom identity and position in the heterocycle, and functional groups attached on the alkyne and N-pyrrole positions. A series of computational studies was performed to provide further insight into the 5-exo and 6-endo dig pathways in these heterocyclic systems. Theoretical predictions were found to reproduce experimental results, highlighting the predictive capabilities of the computations in determining preferred products.

## What happens when you add prey to an Arctic ecosystem? Modelling the apparent competition between snow goose and semipalmated sandpiper

**Sarah Jacques (Université de Moncton)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

Science Atlantic Graduate Research Award, Oral Presentation, First Place

The combined effects of climate change and agricultural intensification have led to an exponential increase in snow geese. Millions of geese migrate annually, in the spring, from agricultural lands to the Arctic generating a massive flow of resources. These additional resources support a higher abundance of Arctic predators. This could be the cause of indirect impacts on other prey species. In particular, this interaction may be one of the causes underlying the recent decline of several shorebirds populations. Indeed, several studies have found that predation risk on shorebirds nests increased near goose colonies. At the same time, shorebirds are less prone to predation during years of high abundance of lemming, the preferred prey of most arctic predators. Despite local empirical evidence of the consequences of snow goose and lemming abundance on shorebirds nest survival, we lack the tools to predict the extent of these impacts at a circumpolar scale. Thus, the main objective of this project is to predict the effect of increasing snow geese populations on the predation rate of a declining shorebirds species' nest, the semipalmated sandpiper. To achieve this, we are currently using parametric differential equations with data from arctic sites with and without goose colonies covering different years of the lemming cycle. Our model will provide a crucial predictive tool to better guide conservation efforts for declining shorebirds species.

## Optimizing sodium dodecyl sulfate depletion via Transmembrane Electrophoresis: Combating Joule Heating

**Philip J. Jakubec (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best undergraduate poster presentation in Analytical Chemistry

Sodium dodecyl sulfate (SDS) is a widely used surfactant favored for its use in protein extractions, solubilisations, and mass-based separation techniques for proteomic analysis. Surfactants interfere with separation techniques and high-resolution detection methods like liquid chromatography and mass spectrometry (MS). Especially of interest to proteomics is that SDS suppresses MS signals resulting in lower resolution data that makes comparison with bioinformatic databases difficult; so, SDS must be removed from samples prior to MS analysis. Transmembrane electrophoresis (TME) is a recently developed system for protein purification capable of depleting >99% of contaminating SDS, while preserving high protein yield >95%. Increasing the strength of the electric field has proven the key to increasing TME SDS depletion rates, but the resulting increase in Joule heating leads to sample losses. Herein, we optimized the design of the TME device and its procedure to mitigate Joule heating, increasing the rate of sample purification three-fold, while maintaining high sample recoveries. TME is a rapid protein purification technique for the frontend sample preparation of proteomic samples for high throughput MS analysis.

## Bis(diarylethynyl-methylene)dihydroanthracenes: Synthesis, properties and tunable aggregation-induced emission

**Matthew A. Johnson (Memorial University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of Science Atlantic Undergraduate Research Award

Aggregation-induced emission (AIE) is a phenomenon in which a class of molecules do not exhibit solution phase emissions but become highly emissive in the solid-state or upon forming aggregates. A newly developed series of molecules, namely, bis(diphenylmethylene)dihydroacenes<sup>1</sup> have been found to exhibit this AIE effect through restriction of intramolecular rotation (RIR) around the phenyl bond, and restriction of intramolecular vibration (RIV) through the acene core. Herein, we examine the effect of extending such structures by an ethynyl unit, ideally they would exhibit a similar crystal packing and therefore undergo a comparable AIE mechanism. However, the extension of the phenyl unit causes lack of steric interactions which makes the RIR mechanism less likely and as a result we obtain differing results. In addition, it would appear that substitution controls the ability of the molecule to exhibit an AIE effect. Finally, attempts to cyclize one of the species to the corresponding tetra-substituted coronene will also be discussed.



# The Development of Butyrylcholinesterase ligands for Diagnosis of Alzheimer's disease

**Kosuke Kanayama (Mount Saint Vincent University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best overall poster presentation in Biological and Medicinal Chemistry

Background: Alzheimer's disease (AD) is the leading cause of dementia. At present, diagnosis involves a subjective clinical evaluation of cognitive function and ruling out other causes of dementia. A definitive diagnosis of AD is subsequently achieved by post-mortem examination of the brain, for pathological hallmarks of AD such as  $\beta$ -amyloid ( $A\beta$ ) plaques and neurofibrillary tangles (NFTs). However,  $A\beta$  plaques and NFTs are also found in many cognitively normal older individuals. Early, definitive diagnosis of AD during life could alter disease management and possibly aid in the development of new therapeutics. In AD, there is an accumulation of butyrylcholinesterase (BChE) activity associated with  $A\beta$  plaque and NFTs in the cerebral cortex, where normally there is low levels of BChE activity. Therefore, BChE may represent an appropriate biomarker for the development of a diagnosis system for AD. **Methods:** The synthesis of targeted iodinated aromatic esters can be achieved by mixing the appropriate alcohol and acid chloride in the presence of triethylamine in a capped reaction vial. The biochemical evaluations can be conducted using UV-vis spectrophotometry. **Results:** An iodinated aromatic ester was successfully synthesized. UV-vis repetitive scans showed that it is hydrolyzed by BChE but not by acetylcholinesterase (AChE). **Conclusions:** The iodinated aromatic ester was successfully synthesized, and its biochemical evaluation showed it is hydrolyzed by BChE but not by AChE. Continuing work involves kinetic analysis of BChE hydrolysis of the ester and its conversion to 123I-labelled product to assess its ability to act as a possible BChE imaging agent for AD in preclinical analysis.

## Temporal stability of genomic differentiation between spawning season components in Atlantic Herring (*Clupea harengus*)

**Quentin Kerr (Dalhousie University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, First Place

Aquaculture & Fisheries Overall Best Paper Award

Atlantic herring (*Clupea harengus*), a vital ecosystem component in the Northwest Atlantic, is the target of the largest pelagic fishery in the region. Complex seasonal spawning and feeding migrations result in intricate and elusive population structure. Herring spawn mostly during two distinct seasons, fall and spring, and significant genomic differentiation has recently been detected between these groups. The present study used a subset of this differentiation, 32 highly discriminatory Single Nucleotide Polymorphisms (SNPs) to answer two questions. First, is this genomic differentiation between fall and spring spawning components temporally stable in the Gulf of St. Lawrence? Secondly, can these SNPs be used as a proxy for spawning season in Bras d'Or Lake herring, where traditional morphological tests might fail? Overall, 276 herring were sequenced and genotyped at these 32 loci. An analysis of molecular variance found no variation in the seasonal differentiation between 2005 (N=90) and 2014 (N=71) in the Gulf of St. Lawrence, suggesting long term temporal stability. Furthermore, a discriminant analysis of principle components assigned 85 Bras d'Or herring to the fall component, and 12 to the spring component, with >99% posterior probability. This large fall spawning presence in the Bras d'Or Lakes likely indicates population change in these herring following the 1999 stock collapse in this region. Overall, this study suggests long-term genetic diversity between spawning components, and demonstrates an application of these SNPs to determine stock structure.

## Fluctuation of Wi-Fi Received Signal Strength Indicator Readings

**Patricia Kibenge (University of Prince Edward Island)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Research Award, Computer Science Oral Presentation, Third Place

Current GPS-based technologies used in smartphones that allow for continuous or frequent localization quickly drain the battery of these devices. A convenient, energy-efficient alternative relies on Wi-Fi Fingerprinting, where a training phase is used to populate a database of locations and corresponding Wi-Fi Received Signal Strength Indicators (RSSIs) before those values are compared to the target location's RSSI values in the locating phase. Crowdsourcing is an efficient way to complete the training phase if this paradigm is used in a large area. The consistency of the RSSIs collected by all devices used in crowdsourcing the training phase is integral to the accuracy of the Wi-Fi fingerprinting method. In addition to dependence on the strength of the signal created by the access point, RSSI levels are dependent on the design of the antenna, which may differ from one device to the next. Research attempted to determine whether a consistent mathematical relationship exists between RSSI readings collected by three different Android smartphones. No reproducible mathematical relationship was found within the results but all smartphones recorded RSSIs that correlated with their distance from the access points, which is essential for this localization method. Therefore, adjusting RSSI values with a mathematical formula is not an acceptable method of RSSI normalization between readings from different devices. However, using Wi-Fi RSSIs for mobile localization is still a viable alternative to GPS.

# The Preparation of Dinucleating Tetraaminodiphenol Supported Bimetallic Bismuth Complexes and their Potential Application Towards the Ring Opening Polymerization of Lactide

**Marcus Kindervater (Mount Allison University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best overall poster presentation in Inorganic Chemistry

The Principles of Green Chemistry, as outlined by Warner and Anastas in 1998, have encouraged an increased emphasis on sustainability within chemical practices.<sup>1</sup> Significant effort has been invested into biocompatible materials, such as poly(lactic acid), as potential alternatives to traditional petroleum-based plastic production.<sup>2</sup> Poly(lactic acid) is a biorenewable and biodegradable polymer that is efficiently synthesized via the ring opening polymerization (ROP) of lactide, which is facilitated by a metal-alkoxide catalyst. In previous studies, dinuclear aluminum complexes have been shown to efficiently catalyze the ROP of lactide with moderate isotactic selectivity under ambient conditions.<sup>3</sup> This study focuses on the synthesis of a dinucleating macrocyclic N<sub>4</sub>O<sub>2</sub>tetraaminodiphenol ligand scaffold to support novel bimetallic bismuth compounds. The synthesis and structural characterization of the macrocyclic ligand scaffold and isolated homo- and heteronuclear complexes will be discussed.

## Defining the role of SOX4/SOX11 during nephrogenesis in vivo

**Morgan King (University of Prince Edward Island)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Communication Award, Poster

Congenital anomalies of the kidney and urinary tract (CAKUT) account for the highest incidence of end-stage renal disease in children. To understand abnormalities in renal development, a greater understanding of nephrogenesis is necessary. SOX genes have been identified to be critical in a number of organogenesis processes, but they have not been extensively studied in the kidney. Previous research has characterized Sox4's importance in the formation of nephrons – conditional ablation of Sox4 resulted in end-stage renal failure. In a complementary study, it was determined that Sox4/11 double knock-out mice die perinatally of renal failure. Analysis revealed a high number of immature nephrons. It was hypothesized that SOX4 and SOX11 cooperatively promote differentiation during renal organogenesis in vivo. Furthermore, it was predicted that the etiology of renal failure/death in Sox4/11 double knock-out mice was due to a primary delay in nephron differentiation, leading to perinatal renal incompetence and subsequent death. To test the hypothesis, a morphometric approach was adopted. Nephrons were quantified in kidney sections using a virtual disector method in 5 different genotypes: Sox4+ /Sox11+ , Sox4HZ/Sox11HZ, Sox4HZ/Sox11KO, Sox4KO/Sox11HZ, and Sox4KO/Sox11KO. Mature glomeruli were quantified at embryonic day (E) 18.5 and postnatal day 21 using a combination of peanut agglutinin staining and haematoxylin & eosin staining. Mature glomeruli were also quantified at E14.5, E16.5, and E18.5 using WT1 immunofluorescence to assess whether there was a primary delay in nephron development. Results demonstrate that SOX4 and SOX11 have important independent roles, but cooperative signaling is required for normal renal development in vivo.

## Earth-Abundant Acid-Stable Electrocatalyst for Water Oxidation Reaction

**Maxine Kirshenbaum (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best graduate poster presentation in Materials Chemistry

The oxygen evolution reaction (OER) is an important obstacle to several industrially-relevant processes, including conversion of CO<sub>2</sub> into value-added materials and clean hydrogen production from water-splitting reactions. In electrochemical cells, the OER proceeds more sluggishly than the cathodic reactions, thereby hindering the performance of the overall cell. Many of the electrocatalysts for the OER are unstable under acidic conditions and/or are cost-prohibitive for large-scale application.<sup>1</sup> Thus, efforts are being made to develop economic and sustainable OER electrocatalysts from Earth-abundant materials.<sup>1-5</sup> Herein, we report the discovery of a material with the lowest overpotential in relation to all other cited Earth-abundant materials. Titanium diboride (TiB<sub>2</sub>) was found to have an overpotential of  $640 \pm 80$  mV. Elemental analysis was performed on the electrolyte and electrode materials before, during and after water electrolysis using inductively coupled plasma mass spectroscopy (ICP-MS), powder X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). Electron microscopy was performed on films prior to electrocatalysis to assess film surface and thickness.

## Utilizing micro-ecological activity against bat pathogen *Pseudogymnoascus destructans* as a means of discovering novel antimicrobial compounds

**Jennifer Kolwich (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of Science Atlantic Science Communication Award

White-nose syndrome (WNS) is an emergent disease in North American bat populations. Since the first documented case in New York just over a decade ago, WNS has spread to 32 states and 7 provinces, leading to population decreases of 90-100% in some sites.<sup>1,2</sup> The causative agent of WNS was determined to be the fungal pathogen *Pseudogymnoascus destructans* (Pd).<sup>2,3</sup> Recent studies that have had success at treating WNS utilize the status of Pd as an invasive species in the skin microbiome of North American bats; they have found that micro-ecological defenses of pre-existing cutaneous specimens could be the key in reducing the effect of the fungus. With this in mind, we have isolated and purified samples of cutaneous microbes from a colony of big brown bats. These purified strains have undergone pairwise assays against a closely related *Pseudogymnoascus* species, as well as Gram-positive and Gram-negative bacteria, to test for inhibitory activity. The metabolites of biologically active strains will be extracted, purified, and tested directly for antimicrobial activity. Fractions shown to have potent biological activity will be analyzed by mass spectrometry and unreported natural products will be characterized.

## Reinventing Porous Silicon Synthesis via Metallothermic Reduction

**Yiqi Lai (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of Science Atlantic Undergraduate Research Award

Porous silicon is an important nanomaterial with wide applications in drug delivery, gas sequestration, energy storage, and photonics. The utility of porous Si is highly dependent on the surface area, crystallinity, morphology, and pore volume, which are often dictated by the synthetic methods used to prepare them. Over the last 25 years, different methods have been developed for the fabrication of porous silicon, but anodic electrochemical etching of silicon wafers in hydrofluoric acid remains the dominant process. As an alternative to this corrosive process, reduction of silica with metals such as magnesium, aluminum, zinc, etc. has been proposed as a less harmful and scalable pathway. This presentation will focus on preparation of porous silicon by the reduction of silica nanoparticles with magnesium and aluminum metals, a process known as metallothermic reduction. The influence of reducing metals, reaction time, and temperature on the crystallinity, porosity, surface area, and structural integrity of porous silicon nanoparticles will be highlighted. Based on these results, optimum reaction conditions to prepare high-surface area porous silicon will be proposed.



## Advances in Ancillary Ligand Design for Enabling Nickel Catalyzed C-N Cross-coupling

**Chris Lavoie (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best graduate oral presentation in Inorganic Chemistry

The palladium catalyzed Csp<sup>2</sup>-N cross-coupling of NH substrates and aryl (pseudo)halides (i.e., Buchwald-Hartwig Amination, BHA), is employed broadly in synthetic organic chemistry for the synthesis of aryl amines and related derivatives. Notwithstanding the broad impact of BHA in basic and applied research, the increasing difficulty for end users to procure precious Pd on larger scales has led to intensified interest into the development of coupling methodologies that utilize inexpensive, non-precious metals. In this regard, nickel has proven to be highly versatile in catalyzing the Csp<sup>2</sup>-N coupling of a broad spectrum of synthetically attractive reagents (e.g., ammonia, alkyl amines, anilines, azoles, amides, etc.).<sup>[1-2]</sup> Despite such advances, our understanding of the influence of ancillary ligand ligation on catalyst performance is currently lacking, which severely impedes the development of superlative Ni catalysts that rival state-of-the-art catalysts from the BHA domain. This inspired a combined experimental and computational investigation<sup>[3]</sup> into the influence of ancillary ligand structure on key elementary steps in conventional Csp<sup>2</sup>-N coupling, which has guided the design of superlative ligand classes based on bisphosphines. The findings of this investigation will be the focus of this presentation, and should provide a useful platform for further ancillary ligand design studies in the context of homogenous nickel catalysis.

## Identifying invertebrate biomonitors and assessing biotransport risk at contaminated historical gold mine sites

**Molly LeBlanc (Saint Mary's University)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

Science Atlantic Communication Award

Gold (Au) mining has been an important part of Nova Scotia's social and economic history since the mid-1800s. There are currently 64 gold districts, containing over 360 gold mines, spread across the mainland. Although many of the mines are long-abandoned, a legacy of environmental contamination remains at most sites. The Au amalgamation extraction process involved using mercury-coated copper plates. Residual waste material, "tailings", often contained elevated levels of mercury (Hg) and was deposited into aquatic environments and wetlands. Additionally, the mined ore was often naturally elevated in arsenopyrite. Therefore, when tailing material was deposited on the surface and exposed to weathering processes, elevated arsenic (As) may also occur. Little work has been done to assess the transfer of Hg and As from tailings to aquatic and terrestrial wildlife. Forming the base of many food webs, aquatic invertebrates play an invaluable role within many ecosystems. However, because they are in direct contact with soil, water and sediment, invertebrates can bioaccumulate significant levels of contaminants, transferring them from sediments to higher trophic levels. The objective of this work was to identify Hg and As levels in invertebrate species, so that they may serve as biomonitors of total mercury (THg), methylmercury (MeHg) and As in impacted wetlands. Additionally, to assess the transfer of contaminants to nearby terrestrial ecosystems via emergent (hatching) insects. Initial findings are presented on bioaccumulation of THg and As in aquatic and emergent invertebrates from impacted wetlands at five historical Au mine sites, and two reference sites.

## Circadian and sex-linked gene expression of melanocortin receptor 5 and androgen receptor in the electric organ of *Brachyhypopomus gauderio*

**Stacey Lee (Cape Breton University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Oral Second Place

Nocturnal weakly electric fish have evolved a unique electric signalling mechanism that allows them to emit an electric signal into the surrounding water to navigate their environment in the dark and to communicate with conspecifics. These fish generate their electric signal via continuous activation of their electric organ, which is composed of specialized electrogenic cells called electrocytes. One species in particular, the gymnotiform electric fish *Brachyhypopomus gauderio*, dynamically modifies the magnitude and timing of its electric signal to avoid predator detection, attract mates, or match its nighttime activity period. These electric signal changes differ between males and females and are mediated at the cellular level by melanocortins and androgens. Yet the specific receptors for these hormones have not been characterized in *B. gauderio*'s electrocytes. For my project, I characterized the sequences for the melanocortin receptor 5 (*mc5r*) and the androgen receptor (*ar*) genes and quantified the expression of these genes in electrocytes sampled from male ( $n=14$ ) and female ( $n=24$ ) *B. gauderio* during the day and the night. I have isolated and localized a complete MC5R and a partial AR sequence in the fully functional form within the electrocytes. Gene expression analysis of *mc5r* and *ar* within the electrocytes is ongoing. By establishing this connection between hormones and electric signal plasticity, I hope to provide further insight into the hormonal control of electrogenic cells.

## Metabolic physiology and environmental tolerances of sablefish (*Anoplopoma fimbria*)

**Robin Leeuwis (Memorial University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Graduate Research Award, Second Place

The sablefish is an emerging aquaculture species on Canada's west coast. However, very little is known about the metabolic physiology of this species, or its environmental tolerances. Such information is important for the industry as the life-history and habitat(s) of this fish differ greatly from that of salmonids, and coastal areas (including those in Canada) are likely to experience increasing water temperatures and/or hypoxic conditions due to accelerated climate change. We used intermittent-flow respirometry to characterize the metabolic response and tolerance of 10 °C-acclimated sablefish (~10 g juveniles and ~660 g adults) to acute incremental decreases in oxygen (10% air saturation/h) and increases in temperature (2 °C/h). Further, we performed identical measurements on adult Atlantic salmon (~1130 g). We used the salmon as a comparative species and given its importance to the Canadian aquaculture industry. Adult sablefish were very hypoxia tolerant [e.g., critical oxygen tension (P<sub>crit</sub>) and O<sub>2</sub> level at loss of equilibrium (LOE) were ~15.5 and 5.4% air saturation, respectively] and could tolerate a maximum temperature (CT<sub>max</sub>) of ~24.9 °C. Both these values were significantly lower as compared to adult salmon (O<sub>2</sub> at LOE ~24.2% air saturation; CT<sub>max</sub> ~26.2 °C), and this is surprising given that adult sablefish and salmon had similar values for routine metabolic rate and aerobic scope. Juvenile sablefish were only slightly less hypoxia tolerant than their adult counterparts (e.g., P<sub>crit</sub> ~18.9% air saturation), however, they had a much higher routine metabolic rate and their upper temperature tolerance was ~2.5 °C lower (~22.6 °C).

## Beyond Episodic Memory: The Role of the Hippocampus in Complex Scene Perception

**Qi Li (Irene) (Mount Allison University)**

Presented at the 42<sup>nd</sup> Science Atlantic Psychology Undergraduate Conference, May 8-9, 2018

Science Atlantic Communication Award, Best Oral Presentation

Even though research to date has revealed a key role for the hippocampus in episodic and allocentric spatial memory, its potential role in non-mnemonic spatial processing remains unclear. To investigate the role of the hippocampus in complex spatial perception, we developed a novel floor plan task: a 2D floor plan of a room was simultaneously-presented with a 3D room scene. Scenes either matched the floor plan (i.e. match), differed by a single missing or added scene element (i.e. single-feature mismatch), or differed by the swapped location of two scene elements (i.e. relational mismatch). Seven healthy older adults (four women,  $age_m = 70.14$  years) and 15 healthy young adults (ten women,  $age_m = 19.27$  years) took part in the study. Due to the hippocampal degradation that typically accompanies normal aging, we hypothesized that older adults would be significantly impaired in forming conjunctive spatial representation only (i.e. match and relational mismatch scene types), compared to young adults. Results revealed that older adults were significantly impaired in the match and single-feature mismatch scenes of the floor plan task, indicating potential flaws in our stimuli design.

## Green synthesis of novel heterosteroids for 2- aminonaphthalenes

**Jun Luo (Acadia University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best undergraduate poster presentation in Organic Chemistry

Synthesis of structurally complex molecules in a short route from readily available starting materials is a challenge in organic synthesis. Therefore, multistep reactions in a domino fashion are being widely investigated by organic chemists. Polyheterocyclic frameworks are very important moieties for the construction of biologically and pharmaceutically relevant molecules. We have developed a highly efficient, transition metal-free, cascade reaction of 2-amino-1-hydroxymethylnaphthalines or 2-amino-1-carboxy-naphthalenes with oxo-acids to produce tetracyclic heterosteroidal framework. It involves one-pot formation of an amide bond, a C-N bond and a C-O bond in tandem. The results obtained thus far will be presented.

# Electrochemical-Surface Enhanced Raman Spectroscopy (EC-SERS) for Bacterial Screening

**Taylor Lynk (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of Murray Brooker Award in Chemistry

The lack of efficiency of current methods for bacterial screening has prompted an increasing interest in developing a cost-effective, rapid, and sensitive alternative for applications in all sectors of society. This project aims to explore a new detection platform for bacterial screening by coupling an applied electric potential with surface-enhanced Raman spectroscopy (SERS); a technique termed electrochemical surface-enhanced Raman spectroscopy (EC-SERS). The goal of using this technique is to improve upon the sensitivity and reproducibility of normal SERS to allow for rapid, point-of-need bacterial detection and identification. This project first shows the EC-SERS characterization of the commonly observed nucleotide breakdown products that dominate the SERS spectra of bacteria: adenine, guanine, xanthine, hypoxanthine, uric acid, 5'-adenosine monophosphate (AMP), and guanosine. This work then concentrates on developing a sample preparation method to be used to study bacteria using EC-SERS for the first time. The results of this project demonstrate the improvement of the SERS spectra for both *E. coli* K-12 and *B. megaterium* bacteria when an electric potential is employed, highlighting the great promise of EC-SERS for use as a fast and affordable bacterial screening method. EC-SERS is also shown to be able to discriminate between the two strains of bacteria by employing a spectral database containing the EC-SERS data for the nucleotide breakdown products.

## Delia species: identification and impact in commercial onion in Nova Scotia

**Maggie MacDonald (Acadia University)**

Presented at the Science Atlantic Environment Conference, March 16-18, 2018

Science Atlantic Undergraduate Research Award, Poster Presentation, First Place

Onion maggot, *Delia antiqua* (Meigen) (Diptera: Anthomyiidae) is considered the predominant *Delia* pest. It is unknown whether *D. antiqua* alone is damaging onion or if it is part of a complex with *D. platura* (Meigen) and *Delia florilega* (Zetterstedt). Objectives of this research are to identify the *Delia* species present in commercial onion fields and quantify the impact of each species on onion development. This project has two components: 1. Commercial field assessments - to determine which *Delia* species are present in commercial onion fields and at what stage of development they are causing damage. 2. Host stage preference assessments - to determine whether *Delia* species (*D. platura* and *D. antiqua*) prefer particular plant growth stages for oviposition and which stages are most impacted by larval feeding under controlled conditions. Results from these experiments have found *D. platura* to have little impact on onion success while *D. antiqua* causes unmarketable damage to onions at all growth stages. Commercial field assessments revealed minimal damage from *Delia* species and the predominant species identified from sticky trap was *D. platura*. Growth chamber studies using *D. antiqua* and *D. platura* are evaluating oviposition preference for onion developmental stages. Although *Delia* flies showed no preference for specific onion stages in the field, results from growth chamber studies suggest that *D. antiqua* females prefer to oviposit on mature onion plants at the 2 true leaf and 5-7 trueleaf growth stages.



## Peaceably Coexisting Armies of Queens Game, and a Variation

**Katie MacEachern (St. Francis Xavier University)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Research Award, Mathematics and Statistics Oral Presentation, Third Place

The Peaceably Coexisting Armies of Queens Game is a two player game in which each player takes turns placing queens on an  $n \times n$  chessboard such that no two queens from opposing armies may attack each other. Play continues in this manner until one player is unable to place a queen, making their opponent victorious. Analysis of this game, which focuses on determining who wins, and in how many moves, shows the First player can always be victorious, regardless of board size. As a game that should always end in a First player victory is uninteresting, a slightly different variation is proposed, that of Peaceably Coexisting Armies of Queens Game with a Single King. This game is played similarly to the original, but on their first move the First player must place a single king that is a member of their army. Analysis of this variation proves to be a more compelling exercise.

## Diet and fattening rates of Semipalmated Sandpipers (*Calidris pusilla*) and Semipalmated Plovers (*Charadrius semipalmatus*) staging in the Acadian Peninsula, New Brunswick

**Hannah Mackellar (Mount Allison University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Oral Third Place

I studied stopover ecology of Semipalmated Sandpipers (*Calidris pusilla*) and Semipalmated Plovers (*Charadrius semipalmatus*) at a previously unstudied staging area in North-Eastern New Brunswick. Birds were captured through mist netting during summer 2017. We collected blood samples from the branchial veins of 33 plovers and 23 sandpipers. I examined diet and fattening rate through stable isotope and triglyceride analyses of blood plasma. This information was then related to data on stopover duration collected using radiotelemetry of tagged migrants. Despite Semipalmated Plovers and Semipalmated Sandpipers exhibiting different bill morphology, they shared similar diets, consisting of a mixture of invertebrate prey and biofilm. However, Semipalmated Plovers had significantly lower average plasma triglyceride concentrations than Semipalmated Sandpipers ( $p=0.009$ ). We found no significant relationship between days before migration and fattening rates in either species. However, fattening rates increased with increasing mass in plovers, meaning that rate of weight gain was exponential. This was not the case in Sandpipers, perhaps because they were gaining weight rapidly throughout their stopover. These data provide novel insight into the diet and fattening rates of migratory Semipalmated Plovers, which have received little study during migration. Moreover, this research supports previous findings that Semipalmated Sandpipers are flexible foragers, consuming different prey than what is eaten elsewhere in their stopover range. Finally, differences among the two species in fattening rate during migratory stopover, notwithstanding their similar diets, suggest that other factors such as migration distance and required fuel loads may affect foraging effort and resulting weight gain for these species.

# The Endocannabinoid System and its Role in the Therapeutic-Like Effect of Stress Controllability

**Victoria Mackey (Memorial University)**

Presented at the 42<sup>nd</sup> Science Atlantic Psychology Undergraduate Conference, May 8-9, 2018

Science Atlantic Communication Award, Best Poster Presentation

The current study provides evidence for a role of the endocannabinoid system in the therapeutic-like effects of stress controllability. Mice were submitted to a behavioural control training paradigm, which was modified after the Morris water maze task, to mimic the recovery of emotional control and cognitive flexibility achieved by psychotherapeutic and behavioural interventions in treatment of depression and anxiety. The chronic mild stress model of depression was used to induce stress-related depressive symptoms in rodents. These effects are reversed by the application of the behavioural control training task, as is evident in the recovery of sucrose preference levels to that of controls and a decrease in despair-like immobility experienced in the forced swim test. AM251, a CB1 receptor inverse agonist, was found to induce anxiety-like behaviours in the elevated plus maze, as well as anhedonia in the fruit loop dig test, suggesting that the endocannabinoid system plays an important role in anxiolytic and anti-depressive effects in stressed animals. The exact role of the endocannabinoid system in the reversal of depressive-like caused by chronic mild stress, through behavioural control training, needs further clarification.

## A Philanthropic Variant of Parallel Chip-Firing

**Maggie MacPhee (Mount Allison University)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Research Award, Mathematics and Statistics Oral Presentation, Second Place

Imagine you have a network representing people and their relationships with one another. Each person initially has some amount of money. Now the richest person, or people, give a dollar to each of their neighbours and then the process is repeated. No money is ever added, which means the system is closed, so it is natural to ask the question: "What is the long term behaviour of the system?" In order to answer this, we must look at the system more formally. If you let each person be represented by a vertex on the graph, you can assign each vertex a finite integral number of chips to represent money. Now, in each round, the vertices with the largest number of chips would "fire" to their neighbours. This is a variant of Parallel Chip-Firing we have called Maximal Chip-Firing. Our primary goal is to look at the long-term behaviour of the Maximal Chip-Firing game on graphs.

## Excited State Proton Transfer Reactions in Polyaryl Phenols

**Jenna McNutt (Acadia University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best undergraduate poster presentation in Organic Chemistry

Electronic excitation of phenols can cause them to become more acidic by several orders of magnitude, and in some cases, can cause the phenolic proton to transfer to basic sites on the same molecule, to produce a phototautomer. These reactions can be very fast and efficient, and have been exploited in the design of sunscreens and laser dyes. In molecules where the basic site is a carbon atom, the phototautomer produced is known as a quinone methide (QM). QMs can subsequently undergo reverse proton transfer, electrocyclization, or addition reactions. It is believed that the most efficient examples of proton transfer to produce QMs require a highly polarized excited state. We are testing this claim by synthesizing highly symmetric polyaryls with two phenol residues, and studying their photochemical reactivity.

# Treatment Efficiency and Stability of Antibiotics in Wastewater

**Katharine Miller (Acadia University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best graduate poster presentation in Analytical Chemistry

The presence of antibiotics and other pharmaceuticals in wastewater is a growing concern. In municipal sewage treatment plants (STPs), antibiotics are only partially eliminated and can therefore be discharged into the environment regardless of wastewater treatment, affecting ecological and potentially human health. Target antibiotics in this research included beta-lactams, macrolides, fluoroquinolones, and triclocarban. An analytical method using liquid chromatography – tandem mass spectrometry (LC/MS/MS) was developed for quantifying these antibiotics. The efficiencies of wastewater treatment technologies used in STPs were determined by analyzing antibiotics in wastewater influents and treated effluents. Various treatment technologies were studied, including primary treatment, modified secondary, aerated lagoon, facultative lagoon, sequencing batch reactor, rotating biological contactors, and oxidation ditch. Further, antibiotic stability was investigated for samples stored in three levels of media: ultra-purified water, treated effluent and wastewater. The experiment was carried out under different conditions: in different non-prefiltered or prefiltered with 0.1  $\mu\text{m}$  filters media stored at fridge temperature and room temperature. It was determined that prefiltration of the samples did not markedly affect the stability of the target antibiotics. Temperature was found to have significant impact on the degradation of antibiotics. The half-lives of antibiotics were inversely related to the storage temperature. It was speculated that fluoroquinolones and macrolides have higher persistence suggested by the concentration asymptote creating favouring conditions for the growth of antibiotic resistant bacteria. The activation energies of antibiotic degradation were calculated. High values of activation energies were found, indicating the antibiotic reactivity was mainly affected by the reaction temperature.

## Effects of PEI Berries blueberry purée on renal oxidative stress

**Emma McDermott (University of Prince Edward Island)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Botany Award, Poster Presentation

Cardiovascular diseases are the leading worldwide cause of death and, along with many other chronic diseases, have been associated with high levels of oxidative stress. Blueberries have been shown to have powerful antioxidant properties, a characteristic crucial for neutralizing reactive oxygen species and reducing the overall level of oxidative stress. PEI Berries Ltd. has patented a new blueberry processing method, called hydrothermodynamic technology, which they claim will allow their purée to maintain more of the blueberries' natural antioxidant properties compared to other processing methods. The objective of my research is to evaluate the bioefficacy of the PEI Berries product. 28 Wistar-Kyoto rats were divided into four feeding groups: a control diet, a control diet with blueberry purée, a high fat diet to induce oxidative stress, and a high fat diet with blueberry purée. It was hypothesized that the blueberry purée would cause a significant decrease in renal oxidative stress, shown by increased levels of antioxidants and related enzymes. Spectrophotometric assays were used to measure glutathione levels and the activity of three antioxidant enzymes. Compared to the control group, the rats fed a control diet with blueberries had a 46.8% increase in superoxide dismutase activity, but this was not significantly significant (Two-Sample T-Test,  $p=0.278$ ,  $n=7$ ). Similarly, there was a 24.9% and 28.1% increase in glutathione reductase and catalase activities, but these were not statistically significant (TwoSample T-Test,  $p=0.118$  and  $0.246$ ,  $n=7$ ). My study has not yet provided evidence that the product is effective at increasing endogenous antioxidants in rat kidneys.

## Investigations of new green catalytic hydrogenations of pinenes

**Ndongou-Moutombi Fanta (Université de Moncton)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best graduate poster presentation in Organic Chemistry

Nowadays, value-added natural products are of great interest in organic synthesis, which justifies the importance of investigating new methods, particularly green ones for their synthesis. Thereby a facile method of selective pinene hydrogenation has been investigated over platinum, ruthenium and rhodium on different supports using green conditions. Reaction time, temperature, catalyst support as well as the transition metal were the different parameters investigated in those reactions. Therefore, our results show that the hydrogenation of  $\alpha$ -pinene over ruthenium on charcoal as support with sonication at room temperature leads to a quantitative conversion to pinanes with a highly selectivity in favor of the cis-pinane. The same result was obtained for hydrogenation of  $\beta$ -pinene with ruthenium over alumina without sonification at room temperature. The Ru/C has been recycled and reused six times with a constant conversion, catalytic activity and selectivity in favor of cis-pinane.



# How Math Anxiety Differs Across Individual Differences in Conceptual and Procedural Knowledge

**Johanna Murphy (Memorial University)**

Presented at the 42<sup>nd</sup> Science Atlantic Psychology Undergraduate Conference, May 8-9, 2018

Science Atlantic Research Award, Best Poster Presentation

Research suggests that there are individual differences in the way children combine conceptual and procedural knowledge. Studies demonstrate that some children rely more on conceptual knowledge, some rely more on procedural knowledge, and some rely equally on both types of knowledge. Additionally, previous research has attempted to determine a factor which can explain the differences between these clusters however, previous attempts have been unsuccessful. The current study investigated whether individual differences in conceptual and procedural knowledge can be explained by math anxiety. Grade 4 students ( $n = 60$ ) and Grade 5 students ( $n = 40$ ) were given measures of conceptual and procedural knowledge as well as measures of math anxiety and general anxiety. The results of this study suggest that both conceptual and procedural knowledge can independently predict math anxiety. However, when both types of knowledge were considered together only conceptual knowledge was a significant predictor of math anxiety. With regard to clusters, the children in this sample demonstrated a three-cluster solution specifically, more conceptual, more procedural, and low on both. However, after controlling for ability, these clusters were not related to math anxiety. These findings provide some insight into the relationship between math anxiety and conceptual and procedural knowledge. Overall, these results suggest that math anxiety is primarily related to conceptual knowledge. Furthermore, the results indicate that any relation between math anxiety and procedural knowledge can be explained by the overlap between conceptual and procedural knowledge. Although, math anxiety does not seem to influence the development of cluster membership.

## Fish movement patterns and habitat suitability in Kejimikujik National Park and National Historic Site

**Brandon Nilsen (Acadia University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Third Place

Aquatic connectivity is vital to the health of fish populations. Brook Trout (*Salvelinus fontinalis*) have specific connectivity and habitat needs due to physiological limitations requiring cold-water temperatures and specific breeding site requirements. Parks Canada is currently considering a plan to construct a physical barrier to limit the inevitable spread of Smallmouth Bass (*Micropterus dolomieu*) and Chain Pickerel (*Esox niger*). These alien invasive species are not currently within the park however they are present in the greater Mersey-Tobeatic (M-T) watershed. When invasive populations invade and become established they have significant negative effects on abundance and diversity of native fish species. The Peskowesk sub-watershed of the M-T watershed is the ideal barrier site to prevent invasion. Therefore, to improve our understanding of fish movements through this site, 244 fishes were tagged in the Peskowesk subwatershed with passive integrated transponder tags and movements were recorded using multi-antenna readers. 32 Brook Trout were detected with certain individuals spending multiple days near antennas. Temperature and dissolved oxygen profiles were recorded to assess presumed summer time cold-water refugia and allow comparison with historical data from 1971 and 2005. Movement patterns of Brook trout within the Peskowesk sub-watershed from historical tagging data (2002–2015) will be used to characterize changes in habitat use. Increased knowledge of current habitat suitability and movement patterns are critical to the decision-making process for potential barrier construction and provide preliminary information for subsequent aquatic monitoring activities.

## Investigation of the DNA binding domain on nickel- responsive regulator Helicobacter pylori's NikR using cysteine mutants

**Tam Pham (University of Toronto)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best overall oral presentation in Biological and Medicinal Chemistry

The study's primary goal is to understand the structural changes of transcriptional regulator NikR in Helicobacter pylori (H.pylori). Using the <sup>19</sup>F-BTFMA chemical tag attached to cysteine residues, we aim to use <sup>19</sup>F-NMR to examine structural changes in H.pylori NikR (HpNikR) at different labelled regions. The mutant T3C, which located on the DNA binding domain, was subjected to this chemical <sup>19</sup>F- tag method. T3C-HpNikR demonstrated similar secondary structure as wildtype. It also showed a higher nickel loading ratio and lower DNA binding affinity than wildtype with the chance of oligomer formation at high concentrations. The labelled <sup>19</sup>F-T3C mutant appeared to lose its oligomerization. Preliminary data of the <sup>19</sup>F-T3C in the <sup>19</sup>F-NMR experiment showed certain correspondence to the cysteine residues; however, peak assignments were not finalized as further supporting data would be obtained in the future.

## A geophysical characterization of a Bog in Gullbridge, Newfoundland

**Joey Pittman Department (Memorial University)**

Presented at the 67th Atlantic Universities Geological Conference, October 26-28, 2018

Best Geophysical Presentation (CSEG Award)

Characterization of a bog near Gullbridge in west-central Newfoundland, was performed with the use of a ground penetrating radar (GPR) and coring. X and Y lines were taken of the bog on snowmobile in two different trips in February 2017 using the Earth Science Department's Sensors and Software GPR with 100 and 250 MHz antennas. The antennas were set up in a sled towed by the snowmobile one person in the back operating the GPR one person operating the snowmobile. The soft and deep snow was troublesome but gave interesting information. Different snowfalls are noted as layering and could possibly be detected in GPR profiles. Processing of the GPR data is done using EKKO Project software by applying many different techniques by observing the Nyquist frequency and applying appropriate filters (highpass, lowpass and bandpass) where applicable. With processing being done in terms of the GPS locations and gain to create the best possible cross sectional view of the area. The aims are to map snow thickness and bog bathymetry and if possible to image structures in both layers. Bog core samples for analysis with the Multiscanner core logger (MSCL). The data from the MSCL will be analyzed and also compared to data collected with the GPR. A bog corer has been borrowed from the geography department. It is planned to test this corer on local bogs, and if the tests are successful, to take core samples of the bog in a final field trip to Gullbridge in November.

## Dibenzothienoisindole dione D-A type organic building blocks

**Jayden T.D. Price (University of New Brunswick)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best graduate poster presentation in Organic Chemistry

Donor-acceptor (D-A) type organic building blocks are currently being pursued as active components to enhance efficiency in various organic electronic devices (OEDs). This work explores the synthesis, derivitization, and characterization of a series of new isomeric D-A type building blocks, composed of maleimide (acceptor) and benzothiophene (donor) moieties, for application in OEDs. With these modifiable scaffolds, properties desirable for commercial applications may be incorporated, such as increased charge mobility and power-conversion efficiency, enhanced thermal, electronic and optical stability, strong light absorption across a broad range of wavelengths, and improved processability. Computational analysis of the target compounds, as well as their optical and electronic properties, will be presented.

## Computational Study of Tetrabenzocoronene Derivatives

**Christopher Qiu (Memorial University of Newfoundland)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CATC best overall poster presentation in Theoretical Chemistry

Tetrabenzocoronenes (TBCs) are polycyclic aromatic hydrocarbons (PAHs) with intriguing structural and photophysical properties. This presentation describes a computational study of TBCs with substituents such as fluorine, chlorine, hydroxide, methoxy, amine, and nitrile groups in the 4,5,14,15 positions (i.e., the “cove region”) based on density functional theory (DFT) calculations. TBCs with these substituents in the 2,7,12,17 positions were also investigated and compared to the “cove” substituted TBCs. The geometries and energies of the TBCs were first optimized and calculated at the ground state, as well as the transition state to evaluate the energy barriers for the isomerization between different possible stereoisomers. The frontier molecular orbitals (FMOs) were also examined to determine the electronic properties of the different TBCs. Nuclear magnetic resonance (NMR) calculations were performed to determine the effect of substitution on the aromaticity of the delocalized system. Time-dependent density functional theory (TD-DFT) calculations were also performed to simulate circular dichroism spectra and determine electronic properties. The results of this study indicated that the geometries of “cove” and “non-cove” substituted TBCs varied due to the steric effects of the substituents and that the energy barriers are significant for the interconversion between the cis and trans isomers so that they can exist distinctly at room temperature.

## Exploration of diastereoselective double alkylation reactions of Grignard reagents with cinnamaldehydes

**Chandika D. Ramful (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC second best undergraduate oral presentation in Organic Chemistry

We have recently observed a novel reaction of a Grignard reagent with 4-fluorocinnamaldehyde. We propose that the reaction results in a diastereoselective double alkylation, leading to two predominant products as indicated by NMR spectroscopy and column chromatography (Scheme 1). The proposed double alkylated product has been characterized. Such a reaction triggers great synthetic interest and is also intriguing from a mechanistic perspective. Our group is now focusing on optimizing the reaction conditions and expanding the scope of the reaction to other Grignard reagents and cinnamaldehydes combinations. Crystallization will be conducted to characterize the products by X-ray crystallography to determine which diastereomer is being produced.

## Development of thymidine analogues as inhibitors of Cps2L

**Alana M. M. Rangaswamy (Dalhousie University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best overall poster presentation in Biological and Medicinal Chemistry

*Streptococcus pneumoniae* is an infectious bacterial strain which has shown high virulence, and resistance towards many antibiotics including penicillin.<sup>1</sup> Cps2L is an enzyme found in *S. pneumoniae*, which is essential to the biosynthetic pathway in building bacterial cell walls. Studies in homologous enzymes such as RmlA have shown that inhibition of the enzyme leads to a marked decrease in virulence and thus pathogenicity of *S. pneumoniae*.<sup>2</sup> The Jakeman group has previously done extensive research towards developing an effective inhibitor of Cps2L, focusing largely on modifying sugars and sugar analogues,<sup>3-5</sup> which act as substrates in the physiological reaction catalyzed by Cps2L (See Figure 1). This project seeks to design and synthesize analogues of thymidine triphosphate (dTTP) as inhibitors, with the intent of improving the fit of the small molecule within the active site of the enzyme. Figure 2 shows two example thymidine derivatives, where the headpiece (phenyl group) may be functionalized in future studies. Synthetic strategies and challenges will be discussed, as well as further variability that may be considered in these structures.



## Effects of the invasive green crab (*Carcinus maenas*) on the American lobster (*Homarus americanus*) fishery in Newfoundland

**Gemma Rayner (Memorial University)**

Presented at the 28<sup>th</sup> Science Atlantic Aquaculture and Fisheries Conference, March 9-11, 2018

Graduate Research Award, Third Place

The American lobster (*Homarus americanus*) is the most commercially important decapod species in Newfoundland. Since the 1990s, fishery landings in Placentia Bay, Newfoundland have been steadily decreasing. The invasive green crab (*Carcinus maenas*) was first recorded in North Harbour (Placentia Bay) in 2007, and during this year lobster landings decreased by 34% compared to previous years. Analyses of the behavioural interactions between the two species around a baited trap were used to better understand the potential impacts green crabs will have on lobsters in the natural environment. Green crabs significantly affected lobster behaviour around a baited trap; when green crabs were present and could freely move around the trap, lobsters approached, attempted to enter and were caught less frequently compared to when no crabs were present. Analyses of predator-prey interactions between adult lobsters and green crabs were also used to determine if lobsters from Newfoundland would recognize green crabs as a potential prey item. It was found that lobsters originating from both Nova Scotia and Newfoundland do actively consume green crabs of all sizes and that the size of the green crab determined the likeliness of it being damaged and consumed by a lobster. The longer a green crab remained in the presence of a lobster the more likely it would be captured and eaten. This research will provide information on the potential impact of green crab on the lobster fishery in Newfoundland and Labrador and can be used by stakeholders in the management of this fishery.

# Investigating the Effects of Gold Nanoparticle Core Size on Ligand Number Density, Phase State, and Mixing

**Katherine Reiss (Mount Allison University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC Physical, Theoretical and Computational Chemistry

The study of self-assembling gold nanoparticles is of great interest due to the unique and often size and shape-dependent electronic, physical and optical properties of the nanoparticles. In general, the mixing of nanoparticles with other media is poorly understood. This is in large part due to the immense synthetic possibilities that allow for variability in nanoparticle sizes and shapes, and the implications this has on the ligand caps—the frontline in nanoparticle mixing. Currently, both ligand density and phase have been shown to have surprising effects on nanoparticle-nanoparticle and nanoparticle-solvent interactions.<sup>1</sup> Although the ligand number density on the nanoparticle surface can be adjusted by choice of the ligand binding motif, the consequent effects on ligand dynamics and phase properties are poorly understood. In this study, a series of nanoparticle core sizes are synthesized in order to investigate the resulting effects on ligand density and mixing with secondary components (solvents). To vary surface curvature we have begun to synthesize a series of spherical gold nanoparticles with core diameters from 5 – 40 nm according to the established synthetic procedure by Jana et al., followed by ligand exchange for a hydrophobic alkanethiol ligand.<sup>2</sup> UV-vis spectroscopy is being used to track the ligand exchange process and analyzed using a re-parametrized DLVO-based model by Wijenayaka et al. to more accurately assess the nanoparticles.<sup>3</sup> X-ray photoelectron spectroscopy will also be used to determine the thickness of the ligand layer. FT-IR spectroscopy of 5nm particles mixed with deuterated alkanes to assess the phase state of the ligand shell will be presented, and applied to the current study.

## Progress toward an asymmetric synthesis of pallescensin-1 and derivatives

**Victoria Rose (Memorial University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC third best undergraduate oral presentation in Organic Chemistry

Furanosesquiterpenoids are a class of structurally diverse natural products containing 15 carbons in total and at least one furan. Pallescensins are a family of furanosesquiterpenoids first isolated in 1975 from the marine sponge *Disidea pallescens*.<sup>1-3</sup> The pallescensin family consists of 10 compounds: three monocyclic compounds with an additional 3-substituted furan named pallescensin-1, -2, and -3, and seven compounds named pallescensins A-G featuring a bicyclic ring system plus a 2,3-disubstituted furan. This work focuses on an expedient synthesis of pallescensin-1 (1). The strategy is centered around a C5-7 bond disconnection which was envisioned to be the most fruitful in terms of devising an asymmetric route toward this molecule. The molecule can thereby be broken down into two coupling partners, a bromofuran (2) and an enone (3), whose synthesis has been completed and will be described. Development of the key copper-mediated conjugate addition of these two coupling partners is underway. Synthetically, we next envision a unified approach to the whole pallescensin family utilizing our key coupling along with more modern selective oxidative cyclization chemistry from our advanced intermediates. The synthetic work described includes synthesis of key intermediates and efforts toward synthesis of the final target via the copper-mediated conjugate addition.

## Investigating dive characteristics of resting and non-resting behaviour in grey seals (*Halichoerus grypus*)

**Milagros Sanchez (Dalhousie University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Undergraduate Research Award, Oral First Place

The study of marine mammal behaviour is typically impeded by the inability to maintain visual observations while the animals are underwater. Recent developments in telemetry technology have allowed researchers to monitor marine mammals beneath the surface, and these tagging techniques have allowed researchers to construct dive profiles for several species of marine animals. Over time, different dive profiles have become linked with specific behaviours, however there is a certain degree of assumption associated with this system. This study focuses specifically on square shaped dives, which are used to estimate foraging effort in several species of marine animals. Tri-axial accelerometers provide additional information on the degree of movement occurring during dive phases when overlapped with dive data. Preliminary results of this study found minimal movement during the bottom phase of some square-shaped dives, suggesting that some square shaped dives are “resting dives”. Head mounted accelerometers, GPS tags and depth loggers were attached to twelve female adult grey seals on Sable Island. Using the data from all three tags, the goal was to identify specific characteristics of resting and non-resting dives (such as bottom duration, maximum depth and descent/ascent rate). Overall, resting dives have a significantly longer bottom duration. Determining other dive characteristics will enable the identification of resting and non-resting behaviour in future and existing data sets, without the use of accelerometers. Square shaped dives comprise of both resting and non-resting behaviour, therefore, square shaped dives should no longer be used as an estimate of foraging effort in marine animals.

## SpaceLaunch: A faster app launcher that supports spatial memory

**Manasi Shah (University of New Brunswick)**

Presented at the Science Atlantic Mathematics, Statistics, and Computer Science Conference, October 12-15, 2017

Science Atlantic Science Communication Award

In this talk, I will describe the importance of spatial memory and our new app launcher that exploits it: 'SpaceLaunch'. Mobile phones have become an essential part of our lives; from managing daily tasks to social connections, from tracking fitness to finding the nearest restaurant or ATM, we depend on mobile applications. With the increasing number of apps, finding our apps is increasingly becoming a problem. At least part of the problem is that app launchers (the interfaces used to find and launch apps) do not support our ability to remember app locations. Current app launchers provide page-based (i.e., apps placed on multiple pages) and folder-based (i.e., apps arranged within folders) mechanisms to access apps. However, these two common interfaces create obstacles to people building their spatial memory. Spatial memory is a form of memory that allows people to remember locations over time and retrieve them quickly. Current app launchers break people's spatial memory by hiding applications inside folders or to the pages which are not visible without slow interactions. To better support the development of spatial memory, we designed an app launcher - called SpaceLaunch - that makes all apps visible at once. Through our study, we found that SpaceLaunch better supports building spatial memory and is faster than other approaches for finding and launching apps.

# Optogenetic modulation of Parvalbumin-expressing interneurons affects mouse primary visual cortex pyramidal cell after-responses

**Jared T. Shapiro (Dalhousie University)**

Presented at the 42nd Science Atlantic Psychology Undergraduate Conference, May 8-9, 2018

Science Atlantic Research Award, Best Oral Presentation

The primary visual cortex (V1) has served as a model brain region for studying cortical information processing because it is the first cortical stage of the visual pathway, and a region where several novel computations arise. Recent work has investigated the neural circuits underlying receptive field properties of mouse V1 neurons because the large genetic toolbox available in this species enables specific cell types to be targeted. One such genetic tool is optogenetics, which has been previously used to demonstrate how distinct classes of inhibitory GABAergic interneurons can affect the excitatory drive of V1 pyramidal cells. Importantly, this past work has focused on optogenetic modulation of the onset and sustained responses of V1 pyramidal cells, but has given no attention to the pattern of activity evoked after photostimulation is terminated. We use optogenetics and in vivo electrophysiological recordings to investigate the role of parvalbumin-expressing interneurons (PV+) in V1 circuitry, and specifically how these interneurons affect pyramidal cell after-responses. We confirm that PV+ activation suppresses the onset and sustained responses of pyramidal cells, and demonstrate that termination of photostimulation produces a “rebound effect” on pyramidal cell activity, which facilitates their after-responses.

## Simple Polyhalide Salts of the Dimethylammonium Cation

**Katrina D. Turrie (Saint Mary's University)**

Presented at the Science Atlantic Chemistry Conference, June 7-9, 2018

Winner of CIC best undergraduate oral presentation in Inorganic Chemistry

A novel  $[(\text{Me})_2\text{NH}_2]_2 [\text{I}_2\text{Cl}_2]$  complex was isolated and characterised using X-ray crystallography. The crystal structure of the dianion,  $[\text{Cl}-\text{I}-\text{I}-\text{Cl}]$ , contains both covalent bonds between the central I2 atoms and halogen-halogen contact bonds between the outer Cl atoms and the diatomic I2 center. This anion has only been reported a number of times and with more complex cations, however, our results show that large cations are not needed for stabilization.<sup>1</sup> Robertson et al., have previously reported salts of the dimethylammonium cation with both the I- and I<sup>3-</sup> anions.<sup>2</sup> In this investigation we have prepared two additional compounds which have been isolated and characterised,  $[(\text{Me})_2\text{NH}_2]_2 [\text{I}_3] [\text{Cl}]$  and  $[(\text{Me})_2\text{NH}_2] [\text{ICl}_2]$ . Given the variety of the anions isolated, our reported salts have the potential to be widely applicable in a number of different technological sectors such as dye sensitized solar cells and electrolytes in batteries.<sup>3</sup>

# A Spectral Analysis of Active Galactic Nuclei

**Sophia Waddell (St. Mary's University)**

Presented at the 37<sup>th</sup> Atlantic Undergraduate Physics & Astronomy Conference, February 2-4, 2018

The Tindall/Steinitz Award in Research, First Place Tie

Active Galactic Nuclei (AGN), are thought to be powered by supermassive black holes which are actively accreting material. AGN demonstrate variability across all wavelengths, including in the X-ray, the emission range studied throughout the project. This presentation will first introduce AGN and explain some classifications. It will follow by examining the X-ray spectral data processed from observations taken by three different satellites; XMM-Newton, Suzaku and Swift. Observations of the radio-intermediate AGN III Zw 2 will be discussed. Various models will be presented for this data in an attempt to explain the inner machinery of these objects. Multi-epoch observations will be used to show the X-ray variability of this object over time. For III Zw 2, spectral differences between observations are critically examined, and it is hypothesized that the spectral variability arises from a precessing jet.



## How does the social environment affect responses to thermal stress in Mangrove Rivulus (*Kryptolebias marmoratus*)?

**Claire West (Mount Allison University)**

Presented at the 48th Science Atlantic Biology Conference, March 9-11, 2018

Science Atlantic Communication Award, Oral

The goal of our study is to investigate the effect of social environment on the response to an acute heat stress in mangrove rivulus (*Kryptolebias marmoratus*). More specifically, we are interested in whether acclimation in isolation or in pairs affects the heat shock response following an environmentally relevant acute thermal stress. Fish were acclimated for two weeks in either pairs or isolation, following which all experimental fish were exposed to an acute heat shock at 39°C for one hour. Additionally, fish in pairs were studied in two groups: full interaction and mesh separation, allowing for chemosensory and visual interaction but not physical interaction in the latter condition. We measured heat shock protein 70 (HSP70) after the environmentally relevant acute thermal stressor, then compared HSP70 levels between the two social conditions. Preliminary data indicates that social condition does not alter the normal heat shock response, but also demonstrates that the degree of interaction within the pairs affects the level of variation in heat shock responses. Further analysis of results will contribute to our understanding of the social-physical environmental interactions in mangrove rivulus (*Kryptolebias marmoratus*).

# Discriminating multiple mineralization events of the diatreme-associated Cu-Mo-W-Au occurrences at the Revenue Deposit, Dawson Range, Yukon Territory, Canada

**Mariah Williams (Saint Mary's University)**

Presented at the 67th Atlantic Universities Geological Conference, October 26-28, 2018

Imperial Oil Best Poster Award

The west-central area of the Tintina Gold Belt, Yukon Territory, Canada, is a perspective area for gold as it hosts large, high-grade deposits such as the Coffee Creek and Casino deposits. The Freegold Mountain Project located in the Dawson Range of the Tintina Gold Belt hosts multiple gold showings, including the Revenue Deposit: a poorly characterized diatreme-associated Cu-MoW-Au occurrence. This thesis project will characterize alteration and ore mineral assemblages at Revenue, and investigate the composition (major, minor, and trace element), and sulfur isotope signatures of ore minerals in order to discriminate different mineralizing events, fingerprint their chemical signatures, and elucidate the processes that led to their formation. Recent field work and sampling of exploratory drill-core confirmed at least two distinct styles of mineralization: early, vein-hosted and disseminated chalcopyrite-pyrite-pyrrhotite associated with potassic alteration in the Revenue Granite, and later breccia-hosted molybdenite-scheelite-pyrite-chalcopyrite with phyllic alteration likely associated with the emplacement of the pyroclastic diatreme and quartzfeldspar-porphyry dykes. Detailed petrographic work using optical microscopy and scanning electron microscopy, in conjunction with short-wave infrared spectroscopy (Terraspec), will i) identify and characterize ore minerals and associated alteration, ii) examine microscopic textures, and iii) quantify the major and minor element composition of the mineral phases. By characterizing the mineral assemblages, we aim to classify the mineralization styles using existing models to be applicable in an exploratory setting. In situ laser ablation inductively-coupled plasma mass spectrometry will be used to determine the trace element compositions of ore minerals, in order to identify unique chemical signatures. Using secondary-ion-mass-spectrometry the sulfur isotope composition of sulfides from different assemblages will be determined. Together with trace element data, this information will provide constraints on the source of sulfur (i.e. mantle or sedimentary derived) and allow for the discrimination of different mineralizing fluids. The results of this study will be used to assign the different mineralization styles at Revenue to existing ore deposit models to benefit exploration programs (e.g., intrusion-related, skarn) in the region.

## An experimental study of the effect of water on chromite saturation in komatiites

**Kate Woods (Dalhousie University)**

Presented at the 67th Atlantic Universities Geological Conference, October 26-28, 2018

The Frank S. Shea Memorial Award in Economic Geology

Chromite is an oxide mineral and the only chromium ore. Economically important deposits of chromite (massive chromitites) are associated with ancient ultramafic magmas known as komatiites. One such deposit has recently been discovered in the Ring of Fire area of the James Bay Lowlands, Ontario. Despite their economic value, the conditions of formation of massive chromitites are poorly constrained. The purpose of this investigation is to characterize the impact of magmatic water on the mineral phase relationships in komatiitic magmas. Orthopyroxene, an important constituent in komatiites, readily incorporates chromium into its crystal lattice. The early crystallization of orthopyroxene therefore inhibits the precipitation of chromite by depleting chromium in the melt. Studies of more felsic systems have shown that magmatic water significantly decreases the crystallization temperature of most silicate phases, but that it has a relatively lesser effect on oxides. Phase equilibrium experiments allow us to test the hypothesis that, by depressing the liquidus of orthopyroxene relative to that of chromite, magmatic water can facilitate the early crystallization and subsequent accumulation of chromite in a komatiitic melt. To accommodate water, experimental charges are sealed in graphite-lined platinum capsules and pressurized to 1 GPa in a piston-cylinder apparatus. This results in fixed pressure and redox state, allowing phase equilibria to be determined as functions of 1. temperature and 2. composition. Preliminary data from this study suggest that water does affect the chromite liquidus, and that olivine may be a heretofore overlooked competitor for chromium. In addition to phase characterization by electron microprobe analysis, we will analyse for chromium and trace element partitioning between mineral phases and melt using laser-ablation inductively coupled plasma mass spectrometry. If trace element partitioning is sensitive to water content, and water content affects the chromite formation capacity of a melt, then such a fingerprint may have applications in characterization of natural komatiites. Komatiites are some of the oldest lavas and best-preserved relics of the Archean Earth. Expanding our understanding of komatiites and their crystallization behaviour could provide important constraints on early Earth processes, including those associated with highly valued ores.