Science Atlantic Atlantique

Student Awards Yearbook

2014-15

Introduction

Science Atlantic conferences provide students with what is often their first opportunity to present their research to an audience of peers and scientists beyond their home institution. This experience has been described by students as invaluable, eye-opening, and rewarding. In these pages, you'll find the photos and abstracts of 84 students from across the region who have excelled in their presentation, research and problem solving skills at this year's conferences. Congratulations to all!

I'd also like to thank this year's sponsors and conference organizers. Without your support, these awards and conferences would not be possible.

Lois Whitehead
Executive Director

2014-15 Conferences

Mathematics, Statistics and Computer Science
October 3-5, 2014
University of New Brunswick, Saint John

Atlantic Universities Geosciences (AUGC)
October 23-25, 2014
University of New Brunswick, Fredericton

Atlantic Universities Physics & Astronomy (AUPAC)
February 6-8, 2015
Mount Allison University

Joint Biology and Aquaculture & Fisheries
March 6-8, 2015
Université de Moncton

Environment
March 13-14, 2015
Saint Mary's University

Psychology
May 18-19, 2015
Memorial University of Newfoundland

Chemistry (ChemCon)
May 21-23, 2015
University of New Brunswick, Fredericton

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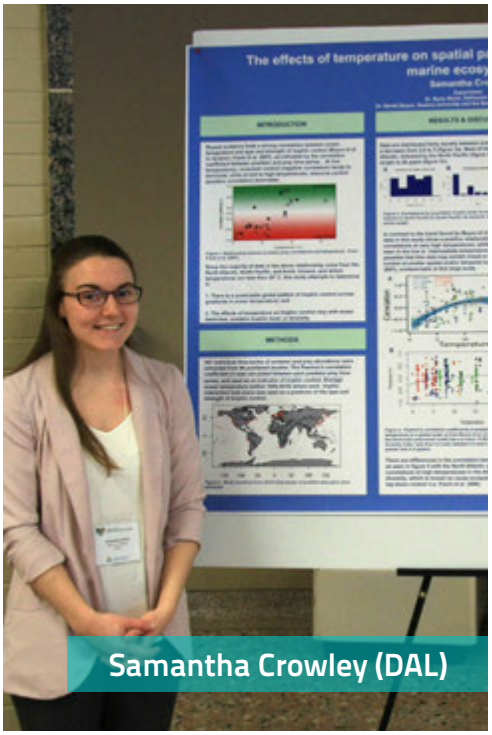


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Krista Latimer (UNB-F)


Haley LeBlanc (SMU)


Rejean Leblanc (MtA)

Science Atlantic Undergraduate Research Award


Mariah Martin Shein (MtA)


Simon Meynell (DAL)


Federico Mora (MtA)


Kathleen O'Donnell (UNB-F)


Zoe O'Malley (UNB-F)


Sasha Power (SMU)


Nicole Ralph (MUN)


Emily Rosta (CBU)


Nicole Shanahan (Grenfell)


Jon Smith (Acadia)


Matt Trace (Acadia)


Matthew van Bommel (Acadia)

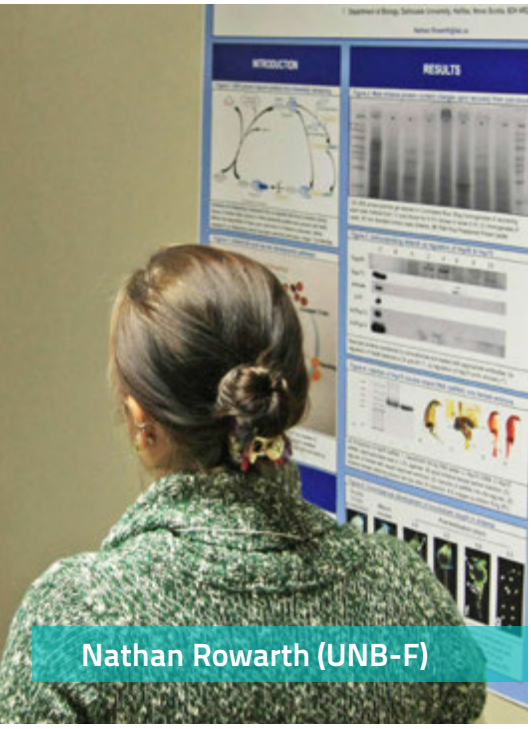

Sarah Van de Reep (StFX)


Nikita Volodin (UPEI)


Yuhuai Wu (UNB-F)

Science Atlantic Graduate Research Award

Alicia Cassidy (UdeM)



Nathan Rowarth (UNB-F)

Marie-France Jones (UNB-F)

Jing Lu (DAL)

Sarah MacLeod (DAL)

Jennifer Murphy (MUN)

Kieran Murphy (StFX)

Graeme Soper (SMU)

AUPAC winners!

Science Atlantic Science Communication Award

Sponsored by Canadian Science Publishing


Michael Buckland-Nicks (SMU)


Laryssa Halat (StFX)


Terri Lovell (MUN)


Kyle Marshall (Acadia)


Emily Peters (SMU)


Tyler Pritchard (Grenfell)


Christopher Small (UNB-F)


Mark Vickers (CBU)

ACEmat Award in Computational Modeling of Materials

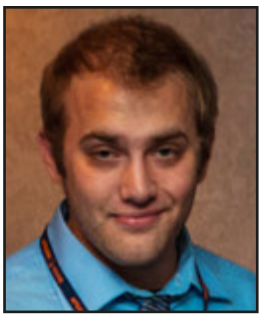

Ernest Awoonor-Williams (MUN)


Hong Yi Shi Yang (DAL)

The ACEmat Award is presented for the best undergraduate presentation using computational methods to study systems of interest to materials science. The award is sponsored by the ACEnet Institute for Materials Modeling and Simulation (ACEmat), part of ACEnet, the high performance computing consortium in Atlantic Canada.

Best Geophysical Presentation

Sponsored by the Canadian Society of Exploration Geophysicists



Andrew Blagdon (MUN)

Dillon White (SMU)

Best Petroleum Geology Presentation

Sponsored by the Canadian Society of Petroleum Geologists

Botany Award

Sponsored by the Canadian Botanical Association

Michael Buckland-Nicks (SMU)

Hardy Strom (UPEI)

Frank S. Shea Memorial Award in Economic Geology

Sponsored by the Mining Society of Nova Scotia

Nikolett Kovacs (MUN)

Frank Shea (1927-1981) was a dedicated career geologist engaged in mineral resources exploration and development in the Atlantic region, including as Chief Geologist in the former Nova Scotia Department of Mines.

K.C. Irving Environmental Science Centre Award

The K.C. Irving Environmental Award is given for the best presentation of undergraduate research relating to the flora or fauna of the Acadian Forest region.

Monique Goguen
(UNB-F)

Joanie Du

Jasmyn Cunningham
(DAL)

Karen Nicholson Award in Neuropsychology

The Karen Nicholson Award is given in honour of **Karen Nicholson** (1971-2007), a former member of the Science Atlantic Psychology Committee, a committed teacher, and a talented and energetic researcher.

ChemCon winners!


bé (MSVU)

Chemical Institute of Canada Awards

Analytical Chemistry


Ceilidh MacDonald (CBU)


Jacquelyn White (SMU)


Julia McCain (Acadia)


Jessica Reiniger (MtA)

Biological/Medicinal Chemistry

Inorganic Chemistry


Leah Bennett (Acadia)


Doug Richards (CBU)


Bright Huo (SMU)


Matthew Tobin (CBU)

Materials Chemistry

Jonathan Cann (UNB-F)

Ifenna Mbaezue (SMU)

Organic Chemistry

Physical, Theoretical, or Computational Chemistry

Zoe Paula (SMU)

Mitch Pinto (Acadia)

Jordan Donahue (UNB-F)

E. Gordon Young Graduate Award for Best Pedagogical Presentation in Chemistry

Eldrid Gordon Young (1897-1976) was an internationally recognized scientist and scholar and the first Canadian to hold the title of biochemist. This award recognizes an outstanding young chemist for his or her teaching and instructional abilities.

Biology Conference winners !

Ricarda Konder
(UNB-F)

Murray Brooker Award in Chemical Education

The Murray Brooker Award recognizes presentations that focus on the student's undergraduate educational experience in chemistry, chemical engineering, chemical technology or chemical technician studies.

Computer Science Competition

Regional division of the ACM International Collegiate Programming Contest

Evan MacNeil

Corinne Madsen

Steve Scott

First: Shellshock (Mount Allison University)

Jessica Blanchard

Alec Gordon

Brandon Smith

Second: Bitshift (University of New Brunswick, Saint John)

Tyler Blair

Raphael Bronfman-Nadas

Alexander Zinck

Third: Dalhousie Gold (Dalhousie University)

About the Computer Science Programming Competition

Science Atlantic coordinates the Atlantic division of the ACM International Collegiate Programming Contest (ICPC), a worldwide, team-based student competition. Tens of thousands of students at almost 2,000 universities from over 80 countries compete each year. The Association for Computing Machinery (ACM) is the world's largest educational and scientific computing society.

Mathematics Problem Solving Competition


Dylan Day

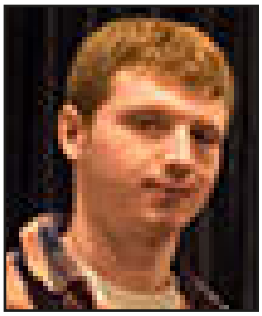

Matthew van Bommel

First: Acadia University

Second: Mount Allison University


John MacMillan


Kathleen MacMillan


Christopher Pardy


Brandon Thorne

Third: Memorial University

About the Mathematics Problem Solving Competition

The Problem Solving Competition is a team-based student competition hosted at the annual Science Atlantic Mathematics, Statistics, and Computer Science Conference.

Abstracts

New Spherical "Core-Shell" Particles for Advanced Lithium-Ion Batteries

Daniel Abarbanel (Dalhousie University)

Presented at the AUPAC2015 (Atlantic Undergraduate Physics and Astronomy Conference), February 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

Lithium-ion batteries power our computers, phones and electric vehicles but there is a desire to improve the operating time and driving range. Positive electrode materials with improved energy density exist, however, they are not stable enough for use in electric vehicles which require thousands of cycles and at least ten years of operational life. A way to overcome this obstacle is to make core-shell materials in which a core with one composition is enclosed in a thin protective shell of another composition in order to develop a long lasting material with enhanced energy density. In this talk, I will describe how core-shell materials were made, characterized and optimized for battery applications.

Is Attentional Vigilance Improved by Listening to Binaural Beats and is it Moderated by Positive Leading Instructions?

T-Jay Anderson (Mount Saint Vincent University)

Presented at the 39th Annual Science Atlantic Psychology Conference, May 18-19, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, poster

The purpose of this study was to test: (a) the popularly-held belief that listening to binaural beats enhances performance on vigilance tasks, and (b) whether any enhanced performance found is due to a placebo effect. Differences in performance were examined by having participants (N = 40) listen to binaural beats, arousal-inducing tones, and white noise while carrying out an Identical Pairs-Continuous Performance (IP-CPT) vigilance task. Half of the participants received positive leading instructions informing them the sounds they would hear were “scientifically proven” to increase attention, awareness, and mental clarity, whereas the other half did not. Listening to binaural beats was not associated with more hits (i.e., correct responses) or faster reaction times (RT) on the IP-CPT compared to listening to the other sound types. Interestingly, the binaural beats and the arousal-inducing tones were associated with more false alarms than the white noise control. With respect to task instruction, the positive leading instructions were associated with significantly lower hit rates than were no leading instructions. These findings suggest binaural beats do not enhance vigilance, and that a positive expectation appears to have a negative effect on vigilance as measured by the IP-CPT. Although inconsistent with popular belief and the scant evidence which supports the enhancing effect of binaural beats on vigilance tasks, the findings suggest that the binaural beats currently being sold as study aids can actually be detrimental to attention when paired with a positive expectation.

Geographic variation in Magnolia Warbler songs

Brianna Burns (Mount Saint Vincent University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, honorable mention, poster

Some species of birds show noticeable variation in their songs; much of this variation is geographic in nature due to copying of song elements from neighbouring male birds. Songs of males from many species of the family Parulidae fall into two categories: A songs (also called repeat or type I) used for attraction of mates, and B songs (also called serial, or type II) used for territorial interactions. The mate attraction function of A songs is hypothesized to constrain their variation because females need to be able to recognize potential mates. Thus B songs are expected to show more geographic variation. This is the first study of the geographic variation in songs of the Magnolia Warbler (Dendroica magnolia). Forty A and B songs from Magnolia Warblers across Nova Scotia (Porter's Lake, Lawrencetown, Cape Breton National Park, Kejimkujik National Park, Taylor Head, and Hartlen Point) were analyzed spectrographically. For the entire song, as well as the first two and last two notes, the duration, and difference between the maximum and minimum frequencies, as well as the number of notes, was measured using Cornell's Raven Software version 1.4. The samples were categorized by song type (A or B) and analyzed by principal components analysis using PRIMER software. Results reveal evidence for geographic variation in the songs of Magnolia Warblers from different parts of Nova Scotia. As predicted, variation was greater among B songs than among A songs.

Applications of Machine Learning on Quantum Chemical Databases: High Accuracy for Low Cost

Andrew R. Cameron (University of Prince Edward Island)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

Machine learning algorithms are employed to discover relationships between elements within large datasets. Progress in applying such techniques to the solution of the non-relativistic Born-Oppenheimer Schrödinger equation has been challenging due to a lack of sufficiently large datasets to afford an exact inductive solution. Recent progress in our group to develop an open, online platform and data repository for computational quantum chemistry has shown promise in addressing this important challenge. As more quantum chemical calculations become accessible, the potential to learn from this data becomes more realistic. In this presentation I will describe our approach to using supervised machine learning in computational chemistry to rapidly generate, optimize, and assess the performance of unique composite methods for determining the non-relativistic electronic energy of a general chemical system. We make use of data from over 270 model chemistries to automatically construct and evaluate 11.9 billion composite methods against a CCSD(T)/CBS benchmark. The performance of our algorithms and the resultant composite methods, as well as a variety of applications will be presented.

Applications of Machine Learning on Quantum Chemical databases: High Accuracy for Low Cost

Andrew R. Cameron (University of Prince Edward Island)

Presented at the AUPAC 2015 (Atlantic Undergraduate Physics & Astronomy Conference), February 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, second place, oral

Machine learning algorithms are typically used to discover relationships between data points within a large data set. This is often usefully applied when there are more equations than there are unknowns. Applying machine learning to quantum mechanics has not always been feasible because large enough datasets have not been available. As more quantum chemical calculations become public and larger databases continue to grow, the potential to learn from data becomes more realistic. This is a statistical approach to find new solutions to the Schrödinger equation. In this talk I will describe our approach to using machine learning in computational chemistry to acquire faster algorithms that use less computational resources while sacrificing as little accuracy as possible. Our approach is to generate composite methods, meaning we will add up previously calculated approximations and weight each component to end up with a result more accurate than any of the components individually.

The effects of temperature on spatial patterns of trophic control in large marine ecosystems

Samantha Crowley (Dalhousie University)

Presented at the Science Atlantic Aquaculture & Fisheries & Biology Conference, March 6-8, 2015

Winner of Science Atlantic Undergraduate Research Award, honorable mention, poster

Marine ecosystems may be structured according to resource availability (“bottom-up” control), or by predation (“top-down” control). Given that top-down control is influenced by the abundance of top predators, a food web community that falls under this type of control should be more susceptible to the effects of overfishing than one under bottom-up, resource-driven control. Recent studies have found that ocean temperature is highly correlated with spatial patterns of trophic control, with resource control dominant in areas of high water temperature (7 to 22 °C), and consumer control dominant in areas of low water temperature (-2 to 7 °C). However, this pattern was observed across temperate and polar northern hemisphere locations and it is uncertain whether there is a predictable pattern of trophic control on a global scale. For this project I am using abundance time-series of marine consumers and their prey extracted from published studies to determine if the previously observed temperature-trophic control relationship is also relevant in tropical and southern hemisphere ecosystems and over the global marine temperature range (~-2 to 32 °C). Understanding the mechanisms influencing these types of trophic control will help identify where they occur, and aid in predicting a community’s response under exploitation and ocean warming.

Self-similar Distributions with Uniform Marginals

Dylan Day (Acadia University)

Presented at the 37th Science Atlantic Computer Science Mathematics & Statistics Conference, October 3-5, 2014

Winner of Science Atlantic Undergraduate Research Award, second place, oral

One way to understand multidimensional probability distributions is to view them in terms of their marginal distributions and their copula, a distribution with uniform marginals that describes the underlying dependence structure between the variables. In certain applications, such as financial risk modelling, these copulas have complicated behaviour that is difficult to approximate with nice functions. One possible solution is to use self similar distributions; these can often appear quite complicated and yet are completely described by a simple method for constructing them, such as an iterated function system or a Markovian operator. This talk will use both methods to produce parameterized families of self-similar distributions that have uniform marginals and thus can be used to approximate copulas.

Global Dimensions of Endomorphism Rings

Brandon Doherty (University of New Brunswick, Fredericton)

Presented at the 37th Science Atlantic Computer Science Mathematics & Statistics Conference October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, fourth place, oral

The global dimension of a ring is defined as the maximum length of projective resolutions of modules over the ring. In this talk, I first discuss background material concerning projective resolutions and Auslander-Reiten quivers. This is followed by discussion of a method for computing the global dimension of the endomorphism ring of a finitely generated Cohen-Macaulay module over a simple curve singularity. This method, developed by Iyama and Wemyss (2010), uses a numbering scheme on the vertices of the universal cover of the singularity's AR quiver to compute approximations of a CM module's indecomposable summands, which can then be used to obtain projective resolutions of the simple modules over its endomorphism ring. Results obtained after implementing this algorithm in Sage are also discussed.

Detection and Quantification of Trace Elements in Rice and Rice Products using X-ray Fluorescence

Kelly Foran (Mount Allison University)

AUPAC 2015 (Atlantic Universities Physics & Astronomy Conference), February 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, second place, oral

Recently, concern about the effect of low-level arsenic (As) exposure over an extended time period has prompted the evaluation of arsenic concentration in foods, especially rice. We set out to use x-ray fluorescence (XRF) to examine the presence and the concentration of arsenic and other trace elements in rice and rice products. A portable XRF analyzer was used to test samples of brown, jasmine, basmati, instant, and microwave rice as well as mixed rice, rice krispies, rice crackers, and brown rice flour. Data from the XRF was used to find amplitude values, in counts, for K, Mn, Fe, Ni, Cu, Zn, and As. Available calibration standards, providing a relationship between sample mass and counts/ppm, were used in converting amplitude values to concentration values for Mn, Zn, and As. Significant concentrations of Mn and Zn were found in most products, and these values were compared to literature. The merit of K, Fe, Ni, and Cu detections was explored by examining observed and expected changes in these elements between different types of rice. The detection limit of the portable XRF system was sufficiently low to detect As in some, but not all, of the rice and rice products.

Prioritizing Catchments for Terrestrial Liming in Nova Scotia

Marley Geddes (Dalhousie University)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, poster

Chronic acidification of freshwater systems is a major issue in South Western Nova Scotia (SWNS). Despite reductions in sulphur emissions, water quality has not improved and is not predicted to improve naturally for another 60 years (DFO, 2013). Acidification is the major limiting factor for the Southern Upland (SU) Atlantic salmon (*Salmo salar*) which were evaluated as endangered by the Committee on the Status of Endangered Wildlife in Canada (COSEWIC) in 2010 (COSEWIC, 2010). Liming, the addition of buffering materials to a freshwater system, is a common method of increasing pH of acidified streams. Similarly, terrestrial liming is the addition of buffering materials to the catchments of the acidified river and is a sustainable mitigative method for acidification. The decision on where to lime and how much to lime is crucial to the success of terrestrial liming. When selecting sites to lime, considerations need to be made for attributes supporting an increasing in pH as well as the ability for a site to support a self-sustaining SU population. There is a need for a comprehensive study in identifying candidate terrestrial liming sites in SWNS. My research will meet this need through a comprehensive GIS analysis of potential sites and the prioritization of these sites using a decision-based model and site scoring methods.

Note on an Approximate Version of Specht's Theorem

Peter Graves-Akerley (Saint Mary's University)

Presented at the 37th Science Atlantic Computer Science Mathematics & Statistics, October 3rd to 5th 2014

Winner of Science Atlantic Undergraduate Research Award, fourth place, oral

We study the problem of how far must the traces of unitary n-by-n matrices with disjoint spectra be. This question is at the root of several recent partial answers to the question "When can we replace an exact condition with an approximate one?" For example, it has been shown, that the equality in the classical Specht condition for unitary equivalence can be replaced with closeness. In this work we show, among other things, that for a fixed pair (*A, B*) of unitary n-by-n matrices with disjoint spectra there always exists a positive integer *k* such that the magnitude of the difference between spectra of A^k *and* B^k and is at least $\sqrt{2n}$. We also show that the result is asymptotically optimal. This enables us to provide some nice new answers to the above question regarding approximate conditions as well as improve the numeric bounds on some previous answers. The research is joint work with M. Bouthillier. It is a continuation of a project that started in the summer of 2013. We would like to thank M. Beattie and M. Mastnak for supervision and financial support.

Skin Shedding in a Marine Plant

Laryssa Halat (St. Francis Xavier University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of Science Atlantic Undergraduate Research Award, first place, oral

Rockweed (Ascophyllum nodosum) is a perennial multicellular brown alga that is a dominant species on rocky shores of eastern Canada. A phenomenon associated with Ascophyllum is the intermittent shedding of the epidermis. The epidermis detaches in patches along the thallus surface, facilitating the removal of colonizing epiphytes and exposing an unfouled surface. A simple method for tracking epiphyte density revealed regular cycles in epiphyte accumulation and epidermal shedding that facilitated investigation at the cellular level. Two hypotheses regarding the developmental stages of shedding were evaluated using a variety of microscopy techniques. To visualize surface topography as well as the structure and appearance of the separating wall, samples of Ascophyllum were viewed with a scanning electron microscope. Thick sections of fixed and embedded epidermis revealed that epiphyte accumulation is accompanied by thickening of the apical cell walls of the outermost layer of cells. Fresh peridermal sections stained with a cell wall dye and a lipid dye revealed the presence of a double cell wall, though the mechanism by which this forms remains unclear. Tissue specimens examined with a transmission electron microscope showed amorphous material devoid of cellular contents embedded between the double cell wall. Evidence from confocal microscopy suggests lipid and membranous material are incorporated into this many layered apical cell wall. The outer and side walls then detach from the underlying meristoderm cells. Thus, Ascophyllum periodically removes biofouling macrophytes, although the composition of the apical cell wall in addition to the factors that trigger this process warrant further investigation.

Determining the Effects of Inhibitors on the Development of Chick Scleral Ossicles in Vitro

Gregory Haller (Mount Saint Vincent University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of Science Atlantic Undergraduate Research Award, third place, oral

The purpose of my research project was to develop a system for culturing embryonic chick eyes in vitro, to determine if it was possible for the eyes to develop outside of the embryo. The main focus of this project was the development of the scleral ossicles within the chick eye; a ring of flat bones that develop through intramembranous ossification. It was found that eyes could survive for four days in a culture containing BGJb medium, while still maintaining a high survival rate. The effects that in vitro culturing had on the eyes varied greatly; some maintaining their shape, some reduced in size, some showed considerable eyelid development, and others showed irregularities in scleral ossicle development. Once it was determined that scleral ossicles could be made to develop in an in vitro culture, inhibitors were added to the cultures in order to observe the effect of global inhibition on the developing chick eye. The inhibitors selected for this experiment were cyclopamine and Noggin, which have been previously determined to affect ossicle development. After experimentation had concluded, the scleral ossicles of eyes that had been cultured in vitro both with and without inhibitor were compared to the scleral ossicles of chicks that developed under normal in ovo conditions. The resulting data is currently undergoing analysis.

Business Failure Prediction for Canadian Charitable Organizations Using Data Mining Techniques

Zhouqin (Mary) He (St. Francis Xavier University)

Presented at the 37th Science Atlantic Computer Science Mathematics & Statistics, October 3-5, 2014

Winner of Science Atlantic Undergraduate Research Award, second place, oral

Business failure prediction has been a classic problem in the business community and a wide variety of data mining techniques have become the new favorites of researchers in the field for their outstanding prediction abilities. While majority of the researches focused on profitable corporations, few attempted to study the charitable sector, especially in Canada, partially due to the lack of available data of this sector. However, this study attempts to apply the existing data mining methodologies on a business failure prediction task aiming at Canadian charitable organizations. Efforts are made to do the prediction with Decision Tree (DT) and Random Forest (RF) methods by a comprehensive use of the panel data containing multiple explanatory variables recorded for thousands of charitable organizations during a three-year period, given that these two techniques are not originally designed for data sets with such complex dimensions. As a result, a novel approach to handle time series attributes using DT and RF by measuring the Dynamic Time Warping (DTW) dissimilarities between observations with respect to particular attributes is presented. In summary, promising prediction results are attained with the best model, generated by the RF method, yielding an overall accuracy of 96.35% and successfully identifying 80.94% of the vulnerable charities. Many interesting variables concerning compensation or expenditure structure of charities are identified as important predictors by both Decision Tree and Random Forest.

Probiotics do not Enhance Anti-Hypertensive Effect of Blueberry Diets in Hypertensive Rats

Zhengcheng He (University of Prince Edward Island)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of Science Atlantic Undergraduate Research Award, first place, poster

Previously we showed that feeding polyphenol-rich wild blueberries (BB) to hypertensive rats lowered systolic blood pressure (BP). Since probiotic bacteria produce secondary metabolites from berry polyphenols which augment the health benefits of berry consumption, we hypothesized that adding probiotics to a BB-enriched diet would augment the antihypertensive effects of BB. Male spontaneously hypertensive rats were fed different AIN93G-based diets for 8 weeks (n=8): Control, 3% freeze-dried wild BB; 1% probiotic bacteria (PRO); or 3% BB + 1% PRO. BP was measured biweekly by the tail-cuff method, and urine was collected twice to determine markers of oxidative stress [8-isoprostanes], nitric oxide synthesis [nitrites] and polyphenol metabolism [hippuric acid (HA)]. Systolic BP at week 8, but not sooner, was lower in the BB and PRO groups (163+5.9 mmHg and 168+6.2 mmHg, respectively) compared to the control diet (188+7.6 mmHg; $p=0.04$). Diet had main effects on diastolic BP at week 8 as well ($p<0.05$). In contrast, the combined BB + PRO diet produced no significant effects on BP. HA excretion, a maker or polyphenol metabolism, was 91% higher after 4 weeks and 74% higher after 8 weeks in BB-fed rats compared to CON ($p=0.0006$). PRO by itself had no effect on urinary HA, and BB+PRO diet did not reduce the magnitude of the BB effect. Excretion of isoprostanes ($p=0.989$) and nitrite ($p=0.373$) did not differ across diet groups. Thus, adding probiotics to a blueberry-enriched diet does not enhance and may impair the antihypertensive effect of BB consumption.

Worm Worries: Anthelmintic Resistance of Worms in Sheep

Kathleen Hipwell (Saint Mary's University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of Science Atlantic Undergraduate Research Award, second place, oral

Gastrointestinal nematodes cause significant morbidity and mortality in sheep. Anthelmintics are essential for worm management, but the sole reliance on these drugs to manage infections has led to widespread anthelmintic resistance. Ivermectin is the only anthelmintic licenced for use in sheep in Canada, although off-label use of benzimidazoles and levamisole is common. In Nova Scotia during 2012, many farmers reported lamb and ewe deaths due to worms, despite anthelmintic treatment. *Haemonchus contortus* has become the most problematic species in Nova Scotia. Closantel, a narrow spectrum drug that kills only *H. contortus*, was accessed through the Emergency Drug Release process. Anthelmintic resistance was investigated through Fecal Egg Count Reduction Testing on nine farms in 2013 and eight farms in 2014. Resistance to ivermectin and benzimidazoles was found on 5/6 and 6/7 farms, respectively. Levamisole was effective on 8/8 farms. Post-treatment larval cultures showed that *H. contortus* was resistant to ivermectin and benzimidazoles, whereas closantel was effective against *H. contortus* and provided adequate worm control for several weeks. Levamisole was effective, but its short period of activity necessitated more frequent treatments. Albendazole in combination with closantel was highly effective against all species, and drug combinations offer a means to extend the useful lifetime of both drugs. To ensure the sustainability of sheep production in Nova Scotia, a transition to using anthelmintic combinations and incorporating alternative non-drug management strategies will be essential.

The Fate of Olivine in the Lower Crust: The Petrology of Coronitic Metagabbro in the Western Grenville Province, Ontario

Jillian Leigh Kendrick (Dalhousie University)

Presented at the Science Atlantic Geosciences Conference, October 23-26, 2014

Winner of Science Atlantic Undergraduate Research Award, first place, overall

The petrology, chemistry, and age of alkaline mafic bodies have been used to differentiate between autochthonous and allochthonous domains in the southwest Grenville Orogen. In allochthons, the characteristic mafic suite is a group of coronitic metagabbros intruded at approximately 1170 Ma. The olivine gabbro protoliths were metamorphosed in the lower crust during the Ottawan stage of the Grenvillian orogeny approximately 1060 Ma. Metamorphism produced spectacular coronitic textures between igneous olivine and plagioclase and other primary minerals. This study examines a 150 m wide outcrop of one such body in the Algonquin domain, recently exposed by highway construction. Petrographic and microprobe analyses on samples collected along the roadcut are underway to determine the metamorphic reactions and P-T conditions the body experienced during Grenvillian metamorphism. This study focuses on metamorphic assemblages overprinting primary olivine. Olivine replacement is ubiquitous in these samples, but was previously undocumented in Grenvillian coronitic metagabbros and remains poorly understood in localities where it exists. Orthopyroxene + ilmenite + magnetite form symplectic pseudomorphs of olivine, separated from relict plagioclase by corona assemblages of orthopyroxene ± clinopyroxene, amphibole ± biotite, garnet + amphibole ± clinopyroxene ± orthopyroxene ± plagioclase symplectite. Preliminary P-T estimates of ≥ 800 ºC and ~12 kb for coronas correlate with P-T estimates from nearby granulite and upper-amphibolite facies gneisses. Determining the reactions responsible for the olivine pseudomorphs and corona assemblages will help constrain P-T conditions and relative timing of their formation, and shed light on the deep crustal processes active during and after gabbro emplacement.

Weak Keys and Plaintext Recovery for the Dhall-Pal Cipher

Karen Korstanje (Mount Allison University)

Presented at the 37th Science Atlantic Computer Science Mathematics & Statistics, October 3-5, 2014

Winner of Science Atlantic Undergraduate Research Award, third place, oral

Cryptography – the study of secure communication – is largely concerned with the design and analysis of ciphers: algorithms which take as input a message to encrypt (called a plaintext) and a secret key and return an encrypted version of the plaintext (called a ciphertext). This summer, my supervisor and I performed a cryptanalytic analysis of the Dhall-Pall Cipher (DPC), introduced by Dhall and Pal in 2010. The DPC is a 128-bit block cipher based on a substitution permutation network (SPN) structure. Due to their similar construction, it can be viewed as an 8-round variant of the Advanced Encryption Standard (AES). However, the round function of the DPC features key-dependent components not present in the AES. A large set of keys render the DPC vulnerable to attack. These "weak keys" introduce significant flaws in the key-dependent portion of the encryption algorithm. Through theoretical analysis and computational verification, we were able to classify a non-negligible portion of the keyspace as weak. Armed with this knowledge, we developed and implemented a number of attacks against the DPC - including two plaintext recovery attacks - which exploit the vulnerabilities introduced by the use of a weak key. The main flaw of the cipher lies in the linear transformation portion of its round function. The transformation is highly regular, with an input byte only affecting the value of bytes to its right. This transformation cannot provide the confusion of data values needed for secure encryption. There is only aspect of the round function which can compensate for the regularity of the linear transformation: a swapping of the two halves of the plaintext. However, this swapping is key-dependent, thus it only occurs in any particular round depending on the value of the key. Should that swapping happen in few or no rounds, the regularity of the transformation carries through the entire round function, and potentially all eight rounds of encryption. Such a property leads to highly predictable output, which makes it easy for an attacker to glean information about the original plaintext. We designed a number of attacks which exploit situations where swapping occurs in few or no rounds. The first set of attacks are distinguishing attacks, which allow us to differentiate between the output of the DPC and that of a random bijection. Based on the success of these attacks, we designed two plaintext recovery attacks. These attacks retrieve part or all of the original message from a ciphertext, provided it was encrypted with a key from one of our classes of weak keys. The second of these two attacks can recover an entire plaintext and is efficient enough to run in only a few seconds on a personal computer. These attacks reveal critical flaws in the design of the DPC. Our work demonstrates that the cipher requires significant review before it is suitable for use in any real-world application.

Effects of Opercular Deformity on Aerobic Capacity in Atlantic Salmon (*Salmo salar*) and Zebrafish (*Danio rerio*)

Krista Latimer (University of New Brunswick, Fredericton)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of Science Atlantic Undergraduate Research Award

Teleosts optimize water flow across their gills by alternating compression and expansion of the cavities anterior and posterior (buccal and opercular, respectively) to the gills. The efficiency of this process relies on three seals, the mouth and two opercular flaps, which allows for the unidirectional flow of water opposite to the direction of blood flow, thereby maximizing the efficiency of oxygen extraction. A fish with short opercula would not have a complete seal, and therefore the efficiency of extracting oxygen could be diminished. This study examined the effects of short opercula on critical thermal maximum (CTMax) of Atlantic salmon (Salmo salar) with naturally short and full opercula, and zebrafish (Danio rerio) with naturally short, surgically shortened, and full opercula. CTMax is a common physiological test that uses increasing water temperature to determine the temperature at which equilibrium is lost, as a proxy for aerobic capacity due to the inverse relationship between water temperature and oxygen solubility. Water temperature was increased by either 6 °C/hour (salmon) or 18 °C/hour (zebrafish) until 36°C, and then by 6 °C/hour until CTMax was reached. General welfare, growth rate, and sex were recorded for all fish, as well as ventricle weight for the salmon. Although statistical analysis has not been completed, there was no obvious indication of opercular condition affecting CTMax in either species. These results provide insight into the perceived diminished aerobic capacity of Atlantic salmon with short opercula.

Polymetallic Co-Ni-As-Bi-Sb-Ag veins in the Southern Slave Province, Northwest Territories

Haley Leblanc (Saint Mary's University)

Presented at the Science Atlantic Geosciences Conferences, October 23-26, 2014

Winner of the Science Atlantic Undergraduate Research Award, first place, poster

Polymetallic ("five metals association") veins containing Co-Ni-As-Bi-Sb-Ag mineralization in the areas of Caribou Lake in the Southern Slave Province, Northwest Territories, Canada, exhibit various stages of mineralization consisting of an early barren (quartz ± ankerite) stage, an intermediate (A) nickel-cobaltarsenide (nickeline ± bismuthinite ± sulfarsenide solid solution [SSS] ± ankerite± quartz) stage, an intermediate (B) sulphide (pyrite ± galena ± chalcopyrite±sphalerite ± ankerite ± quartz) stage and a late (ankerite) stage. The mineralized veins show open-space filling textures containing nickeline rimmed with SSS. This suggests nickeline formed early followed by SSS as S fugacity in the mineralizing solutions increased. Compared to other mineralization sites of this type in the Slave Province (Great Bear magmatic zone) and in other areas (e.g., Cobalt, Ontario) the veins are devoid of native silver and uranium minerals indicating the inability of the hydrothermal fluid to transport these elements, or a lack of these elements in the original source rocks that the fluids obtained their metal endowment from. Stable carbon and oxygen isotope analyses of calcite and quartz in the veins show 13CVPDB ranging from -0.3- 3.3‰ and 18OVMSOW from 12.4-18.1‰, broadly consistent with data from the deposit at Echo Bay, Great Bear Lake but with 13C values in the upper (most 13C-enriched) range reported for all deposits of the Great Bear magmatic zone. Fluid inclusion data from quartz and calcite suggest a NaCl+CaCl2 hydrothermal fluid responsible for metal transport and deposition with salinities ranging between 25.4-36.6 wt%eq. NaCl (absolute: 10.0-19.5 wt% NaCl and 5.8-18.7 wt % CaCl2). LA-ICPMS analyses of single fluid inclusions confirms this and indicates Na:Ca ratios varying widely from one inclusion assemblage to another, ranging from 1.5 to 5.4. The homogenization temperatures for late quartz-hosted inclusions range from 143-196oC and in early calcite-hosted inclusions range from190-256oC. The similar phase ratios in inclusions suggests there was no boiling during ore deposition although the varying salinities, homogenization temperatures, and Na:Ca ratios from one assemblage to another could indicate mixing of two fluid endmembers (e.g., magmatic and meteoric water). Where the polymetallic veins cross-cut the Caribou Lake gabbro, constraints on fluid composition, temperature-pressure of entrapment, and timing are provided. First, a comparison of the chemical composition of fresh and altered gabbros shows that fluid influx caused enrichments in Li-Rb-Cs-Tl-Pb-U-Cu-Ni-Bi-Co-Mo-Ag-Sb, but removed Ba, Sr, Zn and V through the breakdown of feldspars and oxides. LA-ICPMS analyses confirms this showing that the latest stage fluids in the polymetallic veins were highly enriched in K and Ba. Second, primary magnetite-ilmenite intergrowths have been altered to rutile+ankerite in the alteration selvages of the veins. The relative stability of rutile vs. titanite depends on XCO2. Once this is constrained, anaccurate P-T window for the precipitation of alteration stage involving rutile formation can be determined and research is ongoing in this area. Third, a preliminary U-Pb age was obtained from hydrothermal rutile of 1320 ± 80 Ma(discordant). This age has a large error because of Pb contamination from the surrounding country rock but overlaps with the Mackenzie and Berthoud orogenies, suggesting that resetting of U-Pb isotopes occurred during these orogenic periods, or that the mineralized veins themselves formed during these events and are much younger than comparable mineralization styles in the Great Bear magmatic zone.

Counting the Number of Finite Categories with n Morphisms

Rejean Leblanc (Mount Allison University)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, third place, oral

Category theory is a field of mathematics with a high level of abstraction. A category is a mathematical structure made of objects and morphisms. These structures can be very useful tools to other areas in mathematics or even other fields such as computer science. The objective of our research is to count the number of finite categories with n morphisms.

To achieve this we have used various techniques in conjunction with MINION, a constraint satisfaction solver. Previously, the count of finite categories existed for up to 6 morphisms, as seen on the Online Encyclopedia of Integer Sequences. We have obtained counts for 9 morphisms and nearly all counts of 10 morphisms. This research has allowed us to make new conjectures on the behaviors of finite categories.

Assessing Ergonomic and Postural Data for Pain and Fatigue Markers using Machine Learning Tools

Mariah Martin Shein (Mount Allison University)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, third place, oral

Machine learning approaches can be used to identify patterns in postural data that are indicative of workplace fatigue and pain. Two classifiers, C4.5 and MICD, were used to find informative postural features for predicting a participant's fatigue and pain. The presence or absence of pain and fatigue was determined for each participant based on surveys completed after each workstation session. The temporality of the data was expressed by applying a rake (a staged difference in the time of the sample). Each feature was extracted and tested on its own to determine how well a participant's pain/fatigue could be determined with the information contained in that one feature, with higher classification accuracy implying greater information content. The frontal plane of the back was found to be fairly informative, with MICD outperforming C4.5. Further analysis of appropriate rake lengths and C4.5-generated rules is proposed.

Probing the Chiral Magnetic Structure of MnSi Using Hall Effect Measurements and Transmission Electron Microscopy

Simon Meynell (Dalhousie University)

Presented at the AUPAC 2015 (Atlantic Universities Physics and Astronomy Conference, February 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

MnSi is an interesting magnetic material because of the fact that it is able support magnetic solitons known as skyrmions. The magnetic structure of epitaxial MnSi, however, has been surrounded by controversy in recent years. Hall Effect measurements and transmission electron microscopy (TEM) images have been used as evidence for the presence of skyrmions in regions where magnetometric measurements and theoretical calculations suggest none should exist. I will present an explanation for these controversial Hall Effect measurements and unusual TEM images that is consistent with both magnetometry and theory, conclusively resolving some of the big questions about this exciting magnetic system.

EASIK and View Updatability

Federico Mora (Mount Allison University)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, fourth place, oral

Easik is a Java based development kit for EA sketches. Easik allows graphical modeling of EA sketches and views. This information can be converted to SQL code and then saved as a text file, or exported directly to a database. Once exported, Easik supports interaction with the new database, which allows the user to experiment with design decisions. As an extension, this project reviewed the synchronization between sketches and their views. These changes directly dealt with view updatability and the well documented view update problem as well as constraints and their interactions. Users may now safely manipulate data in views while being held to a less restrictive standard than SQL's view definition.

The Effect of Triploidy on Specific Dynamic Action and Basal Metabolism in Juvenile Brook Charr (*Salvelinus fontinalis*)

Kathleen O'Donnell (University of New Brunswick, Fredericton)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, second place, oral

Aquaculture is currently one of the fastest growing food production industries, as it appears to provide an environmentally friendly alternative to harvesting endangered wild populations. However, the productivity, biodiversity, and genetic structure of our waters are now at risk, due to the millions of farmed fish escapees each year. Fortunately, artificially induced triploidy offers a solution that is both environmentally responsible and economically viable, as triploidy renders diploid organisms reproductively sterile. In addition to being sterile, triploids have greater heterozygosity and larger cells in a variety of tissues. Yet on a whole animal level, triploids are very similar to their diploid counterparts. Despite their similarities, the use of triploids in aquaculture has been limited, largely due to their inferior performance if aquaculture conditions are suboptimal (e.g., limited oxygen, space, or food, or high temperatures). The objective of this study was to determine if triploids' inferior performance could be explained by a difference in metabolism, particularly Specific Dynamic Action (SDA), the energy expended to process and store food, and basal metabolism. To answer this, diploid and triploid juvenile brook charr were fed to satiation and then held in respirometers for seven days without food for repeated measurement of oxygen consumption rates at pre-determined time intervals. Preliminary results indicate that triploids have a lower starting metabolism and reach basal metabolism sooner during starvation than their diploid counterparts, though their basal metabolism does not appear to be significantly different.

Using Exuviae to Determine Odonate Population Sex Ratio and Body Size at Emergence

Zoe O'Malley (University of New Brunswick, Fredericton)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winer of the Science Atlantic Undergraduate Research Award, second place, poster

Odonate life histories are intricately tied with the water as well as land, especially during the critical transition from nymph to adult. The purpose of this study was to determine the population sex ratio and the relative body size of each sex at emergence for several Odonate species using exuviae. We collected exuviae over 21 days in May and June 2014 from 12 sites near Grand Lake and along the Saint John River in New Brunswick, Canada. Over 2000 exuviae were collected and the most abundant species of which were Cobra Clubtail (*Gomphus vastus*) and the Stream Cruiser (*Didymops transversa*). Six species that had at least 30 females and 30 males collected were examined for relationships between sex and body size. Female body size was larger than males across the six species. The emergence patterns of the Cobra Clubtail and Stream Cruiser were also examined with various factors that include sex ratio, body size, and distance from water. Using exuviae we can examine Odonate populations without collecting adult individuals, which is important for studying the Skillet Clubtail (*Gomphus ventricosus*), a local species at risk. Examining the sex ratio and body size at emergence can provide valuable information about the population dynamics and life histories of Odonate species.

Post Injury Neuroplasticity in the Cornea

Sasha Power (Saint Mary's University)

Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Undergraduate Research Award, third place, poster

Pain caused by damage to or the malfunctioning of the nervous system has been known to cause severe and disabling pain and is currently considered a challenging clinical problem. This type of pain, called neuropathic pain, is investigated in this study. Specifically, this study attempts to establish a relationship between the pain experienced after an injury to the cornea and the changes observed in the morphology of the neurons as the cornea heals. Furthermore, the relationship between the levels of immune cell infiltration associated with wound healing and the degree of neuroplasticity in the cornea was investigated. The cornea was chosen for this study as it is one of the most densely innervated epithelia in the mammalian body and it is easily accessed by the experimenter. Using mice as a model organism it was determined that immediately following injury the density of nerves in the cornea drops from 62132.0CI±1236.02 µm2/mm2 outside the wound boundary to 38120.5±2523.7 µm2/mm2 inside the wound, severe changes in neuron organisation within the tissue are observed and there was no significant differences in immune cell infiltration when compared to corneas from control animals. Preliminary results show that allowing the cornea to heal for up to 48 hours results in a gradual increase in nerve density over time and seemingly abnormal nerve organisation in the wound site relative to that observed in corneas from control animals. These results suggest neuroplasticity is observed following injury to the cornea.

Investigating the Neuroanatomical Localization of phospho-mTOR in the Hippocampus Following Predator Stress Interactions

Nicole Ralph (Memorial University)

Presented at the 39th Annual Science Atlantic Undergraduate Psychology Conference, May 18-19, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

Traumatic, stressful life events are thought to trigger stress disorders such as post-traumatic stress disorder (PTSD). The animal model, predator stress, recapitulates many of the symptoms of PTSD. Predator stress involves an acute, unprotected exposure of a rat to a cat which causes long-lasting generalized hyper-arousal (manifested as increased startle response) and anxiety-like behaviour (as measured in the elevated plus maze, hole board and light/dark box). Previous research demonstrates that predator stress-induced fear memories is dependent on the kinase activity of the Mammalian Target of Rapamycin (mTOR). Specifically, injection of rapamycin, an mTOR inhibitor, blocks consolidation of predator stress-induced anxiety-like behaviour and hyper-arousal. Although mTOR is critical to the longterm stabilization of fear memory, until now the functional localization of mTOR activity following predator stress was unknown. Thus, the goal of this experiment was to examine activated mTOR (phosphorylated mTOR; pmTOR) in the hippocampus, an area involved in fear processing, following predator stress. We show that predator stress increases pmTOR in all investigated cell lines (CA1, CA3, DG & Hilus) in the dorsal hippocampus compared to controls. Importantly, these results contribute to the understanding of the neurophysiology of fear memories; research with undeniable theoretical and clinical significance.

Existence of Weak Solutions to a Non-Linear Dirichlet Problem

Emily Rosta (Cape Breton University)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, second place, oral

In analysis, it is common to consider the existence of weak solutions to equations which involve the Laplace operator. Often, the weak solutions to such equations live in Hilbert spaces, where results such as the Riesz-Representation Theorem can be easily applied to conclude existence of weak solutions (a well-known example is the Dirichlet problem for Poisson's equation). Proving the existence of weak solutions when working outside of a Hilbert space requires developing an entirely new set of techniques. In particular, my research has focused on weak solutions that live in specific Sobolev spaces that are not Hilbert spaces but rather are reflexive Banach Spaces. As such, I will begin my talk with a brief discussion of background material regarding functional analysis on reflexive Banach spaces. This will lead us to Minty's theorem, the tool I used to conclude the existence of weak solutions to my non-linear Dirichlet problem. Minty's theorem requires that an operator possess four properties: monotonicity, boundedness, hemicontinuity, and almost-coercivity. I will discuss these four properties in detail, making specific reference to the operator in my problem, which is an extension of the p-Laplacian. The p-Laplacian has applications in many areas of the physical sciences, including the study of ice dynamics (a particular example which I looked at during my research).

Other important discussion points will include defining what we mean by a "weak" solution. Using knowledge of weak solutions, I will show how I was able to rephrase my research problem by defining a new operator which provided a condition for identifying weak solutions. I went on to prove (using techniques ranging from Holder's inequality to Lebesgue's Dominated Convergence Theorem) that this operator satisfied the four conditions of Minty's theorem, which tells us that weak solutions to my non-linear Dirichlet problem exist. This original result has been summarized in an existence theorem which I will state in my talk. My conclusion can be applied to prove Sobolev inequalities on large sets, which is currently being carried out by my supervisor Dr. Scott Rodney.

Acoustic Monitoring of Bat Populations in Newfoundland National Parks

Nicole Shanahan (Memorial University, Grenfell)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

White-nose syndrome (WNS) is caused by the fungus *Pseudogymnoascus destructans* and is devastating bat populations throughout eastern North America. There are currently no records of WNS on the island of Newfoundland, but it has been documented on Cape Breton Island and bat populations have not received extensive study and in many areas, bat species diversity and habitat use on the island are not well-documented. Our objectives were to i) use acoustic monitoring techniques to document bat species presence and activity levels in Newfoundland National Parks, and ii) to develop an automated species identification protocol for use on acoustic recordings of Newfoundland bat populations. We deployed bat detectors (SM2BAT+) in Gros Morne and Terra Nova National Parks during the summer and autumn of 2013 and 2014. We analyzed all recordings and identified call sequences to species using manual and automated techniques. We detected three species at multiple sites: *Myotis lucifugus, M. septentrionalis,* and *Lasiurus cinereus*. There was no significant difference between the findings of the automatic and manual call identification protocols ($p=0.08$), although the automated protocol often underestimated the number of *M. septentrionalis* calls detected. Echolocation calls can be recorded to monitor species diversity and habitat use to give a better understanding of current bat population dynamics in Newfoundland.

Tidal Model Validation in the Bay of Fundy

Jon Smith (Acadia University)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, fourth place, poster

Tidal modelling in the Bay of Fundy involves a very large volume of data, and performing comparisons between simulated and observed ocean data has numerous approaches. I will explain my own approach to this validation problem, involving a mix between ocean model validation standards defined by NOAA (National Oceanic and Atmospheric Association) and additional variables for time series comparison. I will also be demonstrating the use of both qualitative graphical analysis and quantitative analysis in determining model performance. Further discussion primarily involves extension of the method to three-dimensional data, and consolidation of the descriptive statistics into a single statistic for more streamlined model run comparisons.

Skolem Labelled Graphs

Matt Trace (Acadia Unviersity)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, fourth place, oral

In many cases, estimating the parameters of a complex computer model can be a difficult task. In this project, we investigate an eleven parameter model for simulating population growth of European red mites whose infestation of apple trees in the Annapolis Valley is of particular interest. We propose using a Gaussian Process (GP) model as a statistical surrogate to the computer model and a sequential design scheme via optimization of the expected improvement criterion in order to efficiently find the set of inputs that correspond to the model response. The suggested approach then simplifies the parameter estimation problem to an inverse problem of a function with a time-series response.

Stage-Wise Surrogate Modeling of Tidal Power Functions

Matthew van Bommel (Acadia University)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

The Minas Passage in the Bay of Fundy has the potential to generate significant power from in-stream tidal energy turbines. A key factor in extracting this power is to determine the optimal locations for these turbines. This process can be seen as finding the (2D) locations which optimize a sequence of (potential) power functions. Gaussian Process (GP) models have been shown to be able to accurately approximate these functions and, compared to using the simulator alone, significantly decrease the required number of computer simulator evaluations. This talk will discuss a “stage-wise surrogate modeling” approach designed to approximate the power functions using GP models and further decrease the total simulator evaluations required to fit an accurate model at each step.

The "Magic" of *Ascophyllum nodosum* Extracts: an Endosymbiotic Hypothesis

Sarah Van de Reep (St. Francis Xavier University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Undergraduate Research award, first place, oral

Three bioassays compared commercially prepared extracts of the brown algae *Ascophyllum nodosum* and *Fucus vesiculosus*. We evaluated the hypothesis that the reported effects of the commercial extracts from *Ascophyllum* are at least partially attributable to fungal metabolites produced by *Mycophycias ascophylli*, a systemic endosymbiont of *Ascophyllum* that is absent in *Fucus*. In a seedling corn growth bioassay, below-ground biomass was enhanced through application of 0.1% and 0.01% *Ascophyllum* extracts. Few differences were observed between the two extract conditions regarding growth rate of shoots and leaves, quantum yield of Photosystem II (PSII) of leaves, and shoot biomass. In a growth experiment with *Lemna minor*, plants grew faster and larger in 0.5% extract of *Ascophyllum*. In addition, the quantum yield and relative electron transport rate of PSII in *Ascophyllum*'s obligate red algal epiphyte, *Vertebrata lanosa*, was significantly higher when maintained in 0.1% *Ascophyllum* extract compared to 0.1% *Fucus* extract. These results support our hypothesis that some of the wide-ranging results of *Ascophyllum* extracts in agriculture are induced by the fungal metabolites in the extract, and not by the chemical composition of the *Ascophyllum* itself.

A Flexible Programming Framework for Multi-Display Environments

Nikita Volodin (University of Prince Edward Island)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, second place, oral

Today, we are surrounded by interactive surfaces, including mobile phones, smart watches, tablets and large touch screen displays. These new devices are changing the way in which we interact with computer applications. However, most of these applications are only designed to work with a single device at a time. This is largely because it is very difficult for application programmers to build applications that allow devices to work together as part of a single application. This means there are many types of applications and many new interaction possibilities that have not yet been fully explored. To address this problem, we have created a framework for building multi-surface applications called WAMS (a Web Application framework for Multi-Surface applications). WAMS reduces the complexity of building multi-surface applications by allowing programmers to focus on application logic rather than on the underlying infrastructure that is needed to allow surface devices to communicate and coordinate. In this presentation, we introduce WAMS, describe its underlying technology and describe how it can be used to simply create powerful new multi-surface applications.

Discrete Equidecomposability and Period Collapse

Yuhuai Wu (University of New Brunswick, Fredericton)

Presented at the 37th Atlantic Mathematics, Statistics and Computer Science Conference, October 3-5, 2014

Winner of the Science Atlantic Undergraduate Research Award, first place, oral

We present new results in two topics related to Ehrhart theory: equidecomposability and period collapse. First, we disprove a conjecture posed by both J. Kantor and T. McAllister that Ehrhart equivalence implies equidecomposablility. We do so by producing two Ehrhart-equivalent denominator 5 triangles and then developing an invariant to show that they are not equidecomposable. Surprisingly, there does exist an infinite equidecomposability relation between these two triangles if we delete an edge. Also, we provide necessary and sufficient conditions for equidecomposability in terms of a family of graphs associated to minimal triangulations of a given polygon. In the other direction, we give an explicit formula for the Ehrhart quasipolynomial in terms of the interior and boundary points up to certain dilates of a polygon. Next, we observe a general linear recurrence relation for the coefficients of the Ehrhart series and give a geometric interpretation for this relation. Under some assumptions, we can do this geometric construction for denominator D triangles with period collapse $k|D$, which converts the period collapse problem into studying half-open rational parallelograms whose discrete and continuous areas are the same. We close with some related conjectures and problems.

Adjustments in Protein Synthesis and Degradation of Starved Arctic Charr (*Salvelinus alpinus*)

Alicia Cassidy (Université de Moncton)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Graduate Research Award, third place, oral

Protein metabolism consists of the interrelated processes of protein synthesis, degradation and growth, which modulates whole-animal growth. In fish, protein metabolism is influenced by external factors such as temperature, pollution and nutrient availability and is under the control of cellular signal transduction pathways. In general, fish have a high capacity to tolerate starvation although there is little information in the literature on the adjustments of signaling pathways during starvation. The objectives of this project are to characterize the molecular mechanisms involved in the control of protein synthesis and degradation in starved Arctic charr (*Salvelinus alpinus*). Various tissues were collected from fish that were fed or starved for 36 days. The fractional rate of protein synthesis was measured using a flooding dose technique. Enzymatic activity of the three major protein degradation pathways (ubiquitin-proteasome, lysosome, and calpains) was measured as well as the activation of cell signaling pathways. This study is the first to measure protein synthesis and the activity of protein degradation pathways in the same fish. Following 36 days of starvation, rates of protein synthesis decreased only in white muscle and liver while there were very minimal effects on protein degradation pathways. The only exception was an increase in proteasome-ubiquitin pathway in the liver of starved fish. Overall, the lysosomal pathway appears to be the primary degradation pathway in muscle protein while the ubiquitin proteasome pathway is predominant in the liver. It is important to measure the adjustments in protein metabolism in order to understand the regulation of whole-animal growth.

Mapping Temporal and Spatial Soil Hydrothermal and Mechanical Properties by Way of the Soil Trafficability Prediction Model (STRAP)

Marie-France Jones (University of New Brunswick, Fredericton)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the Science Atlantic Graduate Research Award, first place, poster

The project deals with the integration of a temporal and spatial model to create an all-inclusive modeling tool to produce soil hydrothermal and forest operation risk maps. The approach taken is modular by connecting temporal hydrothermal processes dealing with soil wetting, drying, freezing, and thawing to spatially anticipated locations of dry versus wet soil drainage conditions. The temporal variations are modeled at daily resolution based on weather data (i.e. temperature and precipitation), and site specific watershed characteristics (i.e. altitude, slope, tree species composition, soil horizon) data via the Forest Hydrology Model (ForHyM). The spatial variations are delivered from LiDAR-generated bare-ground elevation surfaces at 1m resolution by way of a cartographic depth-to-water index (DTW), representing from very poorly drained (DTW100cm) locations. This project utilizes outputs from ForHyM as primary inputs for the Soil Trafficability Prediction (STRAP) model created in ModelBuilder to allow for geospatial forecasting based on specific soil conditions over time. Case study preliminary results focus on North-Western and Central New Brunswick comparing model results with sensor data collected from forest operations machinery and field plot surveys. The machine sensor and field data are used to calibrate STRAP in order to generalize the methodology for weather-dependent and geospatially based forecasting of soil conditions to better enable forest operation planning as seasons change from dry to wet and from wet to dry and from year to year.

Use of *Camelina sativa* Oil and Solvent-Extracted Meal for Atlantic Salmon Fry (*Salmo salar*)

Jing Lu (Dalhousie University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Graduate Research Award, second place, oral

Camelina sativa seed products, including camelina oil (CO) and solvent-extracted camelina meal (SECM), are potentially sustainable feed ingredients for farmed salmonids. The oil has a unique fatty acid profile with 36-39% α-linolenic acid, and the meal has a well-balanced amino acid profile. Atlantic salmon fry (1 g), were fed six diets with either 50 or 100% replacement of fish oil with CO, or 0, 6, 12, or 18% dietary inclusion of SECM for 16 weeks to evaluate the suitability of these novel ingredients. Fish at this early developmental phase are rapidly-growing and highly sensitive to changes in dietary composition. Fish fed 100% CO diet had higher weight gain than fish fed the control, 50% CO and 18% SECM diet (p0.05) was found on the weight gain of fish fed the control, 50% CO, 6% SECM, and the 12% SECM diet. Total feed consumption for fish fed the 18% SECM diet was lower than all other treatments (p0.05) among treatments. Replacing 100% fish oil by CO or up to 12% SECM inclusion can be used in diets for Atlantic salmon fry without affecting growth performance.

Increasing Aluminum Concentrations in Southwest Nova Scotia Rivers from 1980 to Present

Sarah MacLeod (Dalhousie University)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the Science Atlantic Graduate Research Award, first place, oral

Elevated aluminum levels in rivers is known to be toxic for aquatic species, in particular *Salmo salar*; however it was only recently that aluminum has been identified as a potential threat to *Salmo salar* populations in South Western Nova Scotia, Canada (SWNS) (Dennis and Clair, 2012). Previously, it was thought SWNS rivers contained enough Dissolved Organic Carbon (DOC) to render the aluminum in rivers inactive. Key remaining questions are whether aluminum levels are declining following atmospheric pollution reductions, and which months pose a greater threat to *Salmo salar* survival? Here we assess the long term (1980-2011) aluminum concentration trends in three watersheds located in SWNS, as measured by weekly grab samples. This is the first study to quantify aluminum changes in SWNS, and identify any seasonal threats. Our results show that total aluminum levels have significantly increased from 1980-2011 in all three sites. Estimates of ionic aluminum levels indicate that the ionic aluminum concentrations frequently exceed the threshold for the level of aquatic health determined by the European Inland Fisheries Advisory Commission (Howells et al. 1990). This new knowledge that aluminum is at toxic levels and is worsening will have implications for policy on acidification mitigation on SWNS; this is an urgent issue as the local salmon population numbers currently are declining to near extirpation levels.

Green Processing Technologies for the Valorization of Waste Mussel Shells

Jennifer Murphy (Memorial University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Science Atlantic Graduate Research Award, first place, oral

Green chemistry has played a key role in the field of renewable feedstocks, an area of research that has been increasing rapidly over the last decade. (1) Each year in Atlantic Canada there is an estimated 418,000 t per year of waste from fish plants. Waste mussel shells are currently dumped at sea or sent to landfill, which both add a cost to the food processor due to fees that must be paid. (2) The shells cannot be stored because of the residual meat, which attracts vermin. With Canada passing legislation to prohibit dumping waste shells back into our oceans and limited space for landfills, now is the time to look at waste from fisheries and aquaculture as a new source of valuable chemicals.

It is well-known that the shells of molluscs including mussels are primarily calcium carbonate. Calcite and aragonite are the most common forms of calcium carbonate and both are typically present in mollusc shells. The calcium carbonate rich shells have the potential to become high value, low volume products such as a component in cosmetics or low value, high volume products such as high purity calcium carbonate.

This presentation will describe cleaning waste Newfoundland blue mussel shells using environmentally-friendly and easily implemented technologies. The method that has been chosen is biocatalytic, which involves using an industrial protease in water (an abundant and 'green' solvent) to remove the residual protein present on waste mussel shells. The cleaned shells have been fully characterized by a plethora of analytical techniques.

Keep it Fresh and Stay Cool: Combatting *Ciona intestinalis* Biofouling in Aquaculture

Kieran Murphy (St. Francis Xavier University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Graduate Research Award, first place, oral

Since the first recording of *Ciona intestinalis* infestation on a mussel farm in Nova Scotian waters in 1997, this invasive tunicate species has been a prominent disruption to the aquaculture industry, namely causing an increase in operational costs. The rate of proliferation and spread of *C. intestinalis* throughout the province has varied, displayed by the spatial and temporal heterogeneous distribution pattern. It is prosperous in numerous locations, yet it can be entirely absent only a short distance away, and an abundant population can thrive one year, but be scarce the next. The extent to which this unpredictable distribution of *C. intestinalis* is due to nearshore environmental variability is not clear. The aim of this research was to determine the relationship between a range of abiotic variables (temperature, salinity, pH, and water movement) and the abundance of *C. intestinalis. C. intestinalis* abundance and the suite of abiotic variables were recorded at thirteen sites, spanning the entire Atlantic coast of Nova Scotia, from May to October 2014. Multivariate analyses were used to assess relationships between abiotic variables and biofouling communities on a spatial and temporal scale. A complimentary analysis, linear mixed-effects modelling, was used to test the direct relationship between *C. intestinalis* and the abiotic variables. The results suggest that salinity and temperature are the dominant abiotic variables dictating *C. intestinalis* population dynamics. These findings, in addition to 2015 results, could provide valuable scientific information to assist the formulation of future aquaculture management plans.

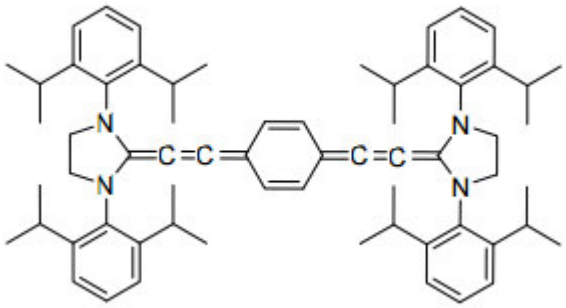
Mono- and Bis-phenylpropargyl imidazolidinium Cations: Structure and Reduction Behavior

Graeme Soper (Saint Mary's University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Science Atlantic Graduate Research Award, first place, poster

Small unsaturated molecules possess both unusual reactivity and spectroscopic features, and in this light they feature prominently in both applied and fundamental organic chemistry. For example, the small fragment $[C_3H_3]+$ exists most commonly as the reactive cyclopropyl cation, and the much more rare species, the propargyl cation $[H_2C\text{-}CC\text{-}H]+$. Unsurprisingly, the extremely unsaturated propargyl cation and corresponding propargyl radical are highly reactive. Here we report the preparation and isolation of a series of phenylpropargyl cations stabilized by *N*-heterocyclic carbenes (**NHC**). The reduction chemistry of these and related molecules has been explored and we have crystallographically characterized the first example of a **NHC** stabilized cumulene. This molecule is exceedingly reactive and this chemistry will be explored. Furthermore, the synthesis, characterization, progress, and challenges will be discussed.



GIS-Based Analysis to Understand the Effects of Environmental Variability on the Growth and Success of Native Plants on Green Roofs

Michael Buckland-Nicks (Saint Mary's University)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the Science Atlantic Science Communication Award, poster

Green roofs have a number of realized benefits including reducing stormwater runoff, saving building energy costs, and reducing the urban heat island effect. However, more research is needed to understand the effects of environmental variability on plants growing in these dynamic systems. In this study, Geographic Information Systems were used in conjunction with statistical analysis to uncover some of these relationships. 69 *Sibbaldiopsis tridentata* plants and 72 *Solidago bicolor* plants were monitored across an extensive green roof located in Halifax, Nova Scotia, from June 5th to November 10th, 2014. Plants were measured based on growth, survival, and reproductive success, and environmental data were also collected. Spatial information was obtained from the plants by turning the roof into a grid system. A 3D model of the roof constructed in ArcGIS was used to generate a solar radiation model and was incorporated into the analysis. Both species achieved faster growth, but had a greater risk or mortality, where there was low vascular plant cover. Plant growth and survival were also greater with higher moisture, lower temperatures, and deeper soil. The data show that significant spatial environmental variability occurred across the green roof system. Furthermore, certain building features created detectable microclimates that influenced many plant and environmental variables. Geographic Information Systems not only provided the ability to visualize important spatial relationships but it also contributed significantly to the data analysis and ultimately to an increased understanding of the dynamic nature of the green roof system.

Skin Shedding in a Marine Plant

Laryssa Halat (St. Francis Xavier University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Science Communication Award

Rockweed (*Ascophyllum nodosum*) is a perennial multicellular brown alga that is a dominant species on rocky shores of eastern Canada. A phenomenon associated with *Ascophyllum* is the intermittent shedding of the epidermis. The epidermis detaches in patches along the thallus surface, facilitating the removal of colonizing epiphytes and exposing an unfouled surface. A simple method for tracking epiphyte density revealed regular cycles in epiphyte accumulation and epidermal shedding that facilitated investigation at the cellular level. Two hypotheses regarding the developmental stages of shedding were evaluated using a variety of microscopy techniques. To visualize surface topography as well as the structure and appearance of the separating wall, samples of *Ascophyllum* were viewed with a scanning electron microscope. Thick sections of fixed and embedded epidermis revealed that epiphyte accumulation is accompanied by thickening of the apical cell walls of the outermost layer of cells. Fresh peridermal sections stained with a cell wall dye and a lipid dye revealed the presence of a double cell wall, though the mechanism by which this forms remains unclear. Tissue specimens examined with a transmission electron microscope showed amorphous material devoid of cellular contents embedded between the double cell wall. Evidence from confocal microscopy suggests lipid and membranous material are incorporated into this many layered apical cell wall. The outer and side walls then detach from the underlying meristoderm cells. Thus, *Ascophyllum* periodically removes biofouling macrophytes, although the composition of the apical cell wall in addition to the factors that trigger this process warrant further investigation.

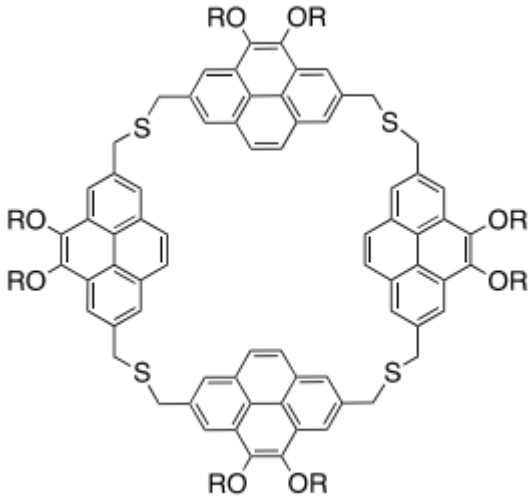
The Synthesis of a Macrocyclic Pyrene-Based Cyclophane

Terri Lovell (Memorial University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Science Atlantic Science Communication Award

When fullerenes are synthesized by laser ablation it results in heterogeneous mixtures of various size fullerenes. Some can separated by dissolution in appropriate organic solvents and purified by column chromatography with alumina columns. Therefore it is of interest to encapsulate currently insoluble fullerenes in order to separate and purify them from heterogeneous mixtures. The presented macrocyclic pyrene-based cyclophane may potentially encapsulate fullerenes which were previously difficult to solubilize and allow for the separation and purification of them.



Physics Beyond the Standard Model: Search for Z' Boson and Dark Photon

Kyle Marshall (Acadia University)

Presented at the AUPAC 2015 (Atlantic Universities Physics and Astronomy Conference), February 6-8, 2015

Winner of the Science Atlantic Science Communication Award

In attempts to better explain dark matter and theoretical predictions by the standard model, it is necessary to introduce new particles into the standard model. The Z' boson and the dark photon are two new particles that we hope will lead to a better explanation of dark matter. By running computational next to leading order scattering simulations and calculations, we are narrowing down the specifics of these new proposed particles in hopes that one day particle accelerators will be able to detect them, much like Peter Higgs did. The talk will begin by discussing the standard model as it is accepted today and the efforts we are going through to expand it as well as our methods of calculation. Finally, current data and results will be discussed and future plans of the research.

Utilization of Growth-Promoters in *Arundo donax*

Emily Peters (Saint Mary's University)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the Science Atlantic Science Communication Award, oral

Arundo Donax is a Mediterranean grass species with synonymous characteristics to an invasive weed, attributing to its viability as a biofuel crop. Historical high growth rate and subsequently high biomass yields without anthropogenic intervention are optimal for a biomass energy crop. The goal of this research is to evaluate whether *Arundo donax* grown on low-quality land can be developed into a new sustainable biomass crop for second generation liquid biofuel production. The objectives are to: 1) identify a method of improving above-ground biomass productivity of *Arundo donax* through inoculation with plant growth-promoters in lieu of synthetic fertilizers and 2) to establish a feasible and low-input approach for *Arundo donax* propagation through in vitro plant tissue culture to reduce production costs and to meet the demand of a large-scale biofuel production system. Diversification of biomass resources is essential to a sustainable biofuel industry.

Exploring the Process of Meaning-Making after Partner Suicide

Tyler Pritchard (Memorial University, Grenfell)

Presented at the 39th Annual Science Atlantic Undergraduate Psychology Conference, May 18-19, 2015

Winner of the Science Atlantic Science Communication Award, oral

Meaning-making is increasingly recognized as a fundamental aspect of the grief experience. This study investigated the process of meaning-making in the narratives of individuals whose partners died by suicide, exploring their meaning reconstruction in response to this form of loss. The narratives of users of a public online grief support forum (n = 50) were analyzed using the Meaning of Loss Codebook (Gillies, Neimeyer, & Milman, 2014), which consists of core categories of meaning of loss in response to the death of a loved one. The results indicated that these individuals predominantly experienced negative affect, a lack of understanding associated with the loss, and a longing for their partners. The grief experience of participants in this study was marked by substantial psychological distress and an ongoing struggle to make sense of and find meaning in this type of loss. It is clear that grieving the loss of a partner as a result of suicide presents unique challenges to meaning-making in comparison to other types of loss. Given the importance of this aspect of adjustment to loss, these findings deepen the understanding of this component of grief and inform the provision of support for those grieving a loved one who died by suicide.

Zebrafish haematology – What Can be Done with 2 µl of Blood?

Christopher Small (University of New Brunswick, Fredericton)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Science Atlantic Science Communication Award

The rise of the zebrafish as a model organism has been rapid, however, this surge in popularity has not been equal in all branches of research. The zebrafish has become prevalent in the fields of development, genetics, and biomedical research, but it has lagged in the physiology and aquaculture research communities. This lag is largely driven by the small size of the fish limiting the amount of tissue that can be sampled, especially when non-lethal sampling is required. Recent work has suggested that up to 2 µl of blood can be collected weekly from adult zebrafish non-lethally without inducing complications due to anaemia. This leads us to the critical question that must be answered before the zebrafish becomes a mainstay in haematology research: What can be done with 2 µl of blood? The strength of the zebrafish model comes from its fully sequenced genome, well-established and customizable techniques, and a wide array of readily available transgenics. In this talk, I will discuss some the techniques that I have been developing to overcome the small-size limitation to allow physiology and aquaculture researchers to take advantage of the power of the zebrafish model.

Student Perceptions of Mental Health, Services & Supports: A Grounded Theory Study

Mark Vickers (Cape Breton University)

Presented at the 39th Annual Science Atlantic Undergraduate Psychology Conference, May 18-19, 2015

Winner of the Science Atlantic Science Communication Award, oral

Young adults attending university are estimated to report mental illness twice as often as other individuals their own age (Heck et al., 2014). Despite the fact that mental health is a major issue in the university setting, many postsecondary institutions are cited as having a hands-off approach when it comes to dealing with mental illness (American College Health Association (ACHA), 2010; Gray, 2007). Furthermore, it appears that a large majority of students are unaware that these services even exist (Yorgason et al., 2008). At present, there is a lack of research involving the student voice in determining barriers to help seeking among the student population and in the discussion of ways to address, and to develop solutions for, these issues. The current study conducted 18 semi-structured interviews with a diverse sample of Cape Breton University (CBU) students in regards to their perceptions of the climate of mental health on campus. Using Grounded Theory Methodology, the research team determined four primary barriers related to seeking help at the mental health services available to students on and off campus. As well, using the perspective of the student sample, the current study proposes four possible solutions as to how to improve the climate of mental health on campus.

Computational Prediction of Cysteine pK_a's

Ernest Awoonor-Williams (Memorial University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2105

Winner of the ACEmat Award in Computational Modeling of Materials

The amino acid cysteine serves several unique roles in chemistry and biochemistry because of the chemical reactivity of the thiol group (S-H bond) in its side chain. This reactivity has been exploited by pharmaceutical chemists and drug developers in designing anti-cancer drugs that can bind covalently to their target by undergoing an electrophilic addition to a cysteine thiol. Cysteine's reactivity towards a drug molecule depends on its acidity, a property quantified by a pK_a value. A cysteine with a low pK_a will be more reactive towards electrophilic inhibitors. Experimentally identifying a targetable cysteine residue and determining its pK_a is a difficult task because of the need to express and purify the protein and the presence of many ionizable groups in a protein. We have evaluated the PROPKA, MCCE and H++ methods for estimating protein side chain pK_a's and found that these methods perform poorly for predicting the pK_a of cysteine residues. We are developing replica exchange free energy perturbation methods for calculating cysteine pK_a's using all atom molecular dynamics simulations within GROMACS. This method provides a more rigorous approach for calculating pK_a's. We are using these methods to identify reactive cysteine in the active sites of human protein kinases that are potential targets for covalent-modifier drugs.

Simultaneous Optical Control of Exciton Qubits Confined to Two Semiconductor Quantum Dots via Femtosecond Pulse Shaping

Hong Yi Shi Yang (Dalhousie University)

Presented at the AUPAC 2015 (Atlantic Universities Physics and Astronomy Conference, February 6-8, 2015

Winner of the ACEmat Award in Computational modeling of Materials

Optimal quantum control is a process by which one can achieve a target final quantum state of a quantum system through iterative adjustments to the control Hamiltonian. This can be achieved using femtosecond pulse shaping, by which the phase and/or amplitude of the pulse may be controlled. In addition to the optimization of general physical processes such as chemical reactions products and nonlinear optical signals, this approach has recently been applied to optimizing parallel single qubit gates in multiple semiconductor quantum dots. In this work, we apply numerical pulse optimization techniques to explore multi-qubit manipulation as a function of the electronic structure parameters of the quantum dots. We show that numerically optimized pulses operating on exciton qubits produces high fidelity quantum gates for a range of dipole moments, transition frequencies, and arbitrary initial and final states. This work enhances the potential for scalability by reducing the laser resources required to control multiple qubits.

A Ground Penetrating Radar Study of Bogs and Lakes in the Howley Basin, Newfoundland

Andrew Blagdon (Memorial University)

Presented at the Science Atlantic Geosciences Conference, October 23-26, 2014

Winner of the Best Geophysical Presentation

This study involves conducting ground penetrating radar surveys over bogs and lakes in the Howley Basin in western Newfoundland under the supervision of Dr. Alison Leitch. As a result, physical properties of the lakes and bogs such as the nature of the base contact were properly determined and used to make inferences about the Howley Formation rocks underlying them. There is a widespread interest in the Howley Formation rocks because of the presence of a Carboniferous pull-apart basin that may accommodate undeveloped hydrocarbons. Overall, the purpose of this research is to increase understanding of the basic nature of bogs and lakes in the area since they cover much of the geology, particularly that of the Howley Basin. Ground penetrating radar emits electromagnetic pulses into the subsurface and detects reflections from objects and interfaces with contrasting electrical properties. The depth range of ground penetrating radar is limited to a few tens of meters, making it a suitable survey technique for imaging bogs and shallow lakes. The signal penetration depth is limited by attenuation (energy loss) due to the conductivity of the ground and to signal scattering. Although attenuation is high in lakes and bogs there is little scattering, with a strong contrast in electrical properties at their bottom interfaces, making ground penetrating radar the ideal technique for imaging the base of lakes and bogs.

Variation in Style of Overpressure in Scotian Shelf Wells, Scotian Basin

Dillon White (Saint Mary`s University)

Presented at the Science Atlantic Geosciences Conference, October 23-26, 2014

Winner of the Best Petroleum Geology Presentation

Overpressure is a phenomenon where pressures greatly exceed normal hydrostatic pressure and occurs in many wells within the Scotian Basin. Due to this area being actively explored for oil and gas over the last five decades, it is very important to understand where and what is causing overpressure. The main causes of overpressure are disequilibrium compaction, clay diagenesis, and hydrocarbon generation, although, the relative importance of these processes in the Scotian Basin is uncertain. To assess and interpret the causes of variability in the style of overpressure in different wells in the Scotian Basin, velocity and density data from wireline data logs were used to produce velocity vs. density cross plots. These plots allowed the possible secondary mechanisms of overpressure generation to be visualized. XRD of < 2 μm clays from shales within overpressured wells were analyzed based on clay mineralogy to possibly find a link between overpressure and diagenesis occurring in the studied samples. The method of cross plot analysis does indeed work for finding patterns of velocity vs. density changes below overpressure. Down-Well variation in velocity vs. density of shales based on wireline logs showed a wide range of velocity vs. density patterns in overpressured sections. There was an apparent regular distribution of different types observed based on velocity-density patterns. Fractures and cementation may have an influence on velocity and density downwell. The fractures may be due to the buildup of overpressure and its eventual release. The opening of fractures would cause a decrease in velocity and that would be observable in velocity-density plots.

GIS-Based Analysis to Understand the Effects of Environmental Variability on the Growth and Success of Native Plants on Green Roofs

Michael Buckland-Nicks (Saint Mary`s University)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Botany Award, oral

Green roofs have a number of realized benefits including reducing stormwater runoff, saving building energy costs, and reducing the urban heat island effect. However, more research is needed to understand the effects of environmental variability on plants growing in these dynamic systems. In this study, Geographic Information Systems were used in conjunction with statistical analysis to uncover some of these relationships. 69 *Sibbaldiopsis tridentata* plants and 72 *Solidago bicolor* plants were monitored across an extensive green roof located in Halifax, Nova Scotia, from June 5th to November 10th, 2014. Plants were measured based on growth, survival, and reproductive success, and environmental data were also collected. Spatial information was obtained from the plants by turning the roof into a grid system. A 3D model of the roof constructed in ArcGIS was used to generate a solar radiation model and was incorporated into the analysis. Both species achieved fastest growth, but had a greater risk of mortality, where there was low vascular plant cover. Plant growth and survival were also greater with higher moisture, lower temperatures, and deeper soil. The data show that significant spatial environmental variability occurred across the green roof system. Furthermore, certain building features created detectable microclimates that influenced many plant and environmental variables. Geographic Information Systems not only provided the ability to visualize important spatial relationships but it also contributed significantly to the data analysis and ultimately to an increased understanding of the dynamic nature of the green roof system.

Analysis of the Salt Pan Marine Fungal Community

Hardy Storm (University of Prince Edward Island)

Presented at the Science Atlantic Aquaculture & Fisheries and Biology Conference, March 6-8, 2015

Winner of the Botany Award, poster

Decomposition and nutrient cycling play a vital role in salt marsh ecology. Natural soil depressions in marsh systems create ecologically distinct microcosms, called salt pans, where adapted species such as the marine macrophyte Ruppia maritma thrives in the dynamic salinity of the pan. As primary decomposers of plant material, distinct fungal communities thrive in these small pockets of marsh, tolerating the changing saline conditions and using available metabolic resources in the microcosm. Although salt marsh fungi have been studied intensively, especially saprophytes of Spartina alterniflora, a fungal catalogue of species specifically associated with the salt pan, including saprophytes of Ruppia have not been documented. To identify key fungal species involved in the decomposition of cellulose within the salt pan microcosm, fungal isolates were obtained from submerged and senescent plant material (of Ruppia maritma and Spartina alterniflora) along with pan sediment. Fungal isolates were identified using micromorphology and sequencing the ITS rDNA barcoding gene and evaluated for their ability to degrade cellulose over a range in salinity. By assessing the source and rate of occurrence of fungal isolates from the various substrata along with their ability tolerate and actively degrade cellulose at various salinities, the specific ecological roles of the isolated fungi was inferred, providing insight into the role of the various fungal species within the salt pan community.

Carlin-Style Gold Mineralization in the Yukon Territory, Canada; Venus Zone, Einarson Property

Nikolett Kovacs (Memorial University)

Presented at the Science Atlantic Geosciences Conference, October 23-26, 2014

Winner of the Frank Shea Memorial Award in Economic Geology

Carlin-style deposits are broadly categorized as a sediment- (predominantly carbonate-) hosted class, with gold contained as solid solution or submicron particles within disseminated pyrite and arsenian pyrite. To date, Carlin-type gold deposits have been largely defined and described in the Great Basin region of Nevada. However, recent discoveries in the Yukon Territory show many of the defining characteristics of Carlin-type gold deposits. The Einarson Property is located in the central eastern part of the Yukon Territory at 64° 0' N, 131°57' W - 15 km east from the 50 km long Nadaleen Trend, which hosts six recently recognized zones of Carlin-type mineralization in Middle Proterozoic to Middle Paleozoic carbonates of the Selwyn Basin. The 1.65 km^2 Venus Zone is located on the northwest side of the Einarson property, where initial drilling has intersected values as high as 9.67 g/t Au over 38.7 m within silicified, sandy dolostone. This honours project is designed to compare the Venus Zone to the Carlintype deposits and environments in Nevada. Thin section analysis, SEM-EDX-MLA and a compilation of field and exploration geochemical data will be used to further elucidate the ore paragenesis, deportment and localization of gold mineralization of the Venus Zone. This will form the basis for the comparison of this example, within an emerging gold district in the Northern Cordillera, with the classic examples and characteristics described from the Nevada districts of Carlin-style mineralization.

Modelling and Mapping Bryophyte Distributions in New Brunswick using a Depth-to-Water Index

Monique Goguen (University of New Brunswick, Fredericton)

Presented at the Science Atlantic Environment Conference, March 13-14, 2015

Winner of the K.C. Irving Environmental Science Centre Award

Plant species composition is known to vary along environmental gradients. Bryophytes such as Sphagnum moss grow in abundance where water remains near the surface year-round, while others (i.e., *Dicranum polysetum*) prefer mesic locations. This project uses a cartographic depth-to-water (DTW) index to model the potential distribution of common moss species of New Brunswick at a landscape scale. The DTW index quantifies changing soil drainage conditions across the land at 1m resolution, from very poor (DTW100cm). The index is created using digital elevation models derived from airborne LiDAR data. Moss species composition and relative abundance of 12 species were measured along transects traversing the landscape, from wetlands to uplands. Patterns of bryophyte species abundance and occurrence are quantified using regression models, and habitat suitability maps are created in ArcGIS, relating species composition to environmental variables such as DTW, vegetation type, and canopy closure. In general, the moss species are found to sort along a moisture gradient, with a higher frequency of hydrophytic mosses found in lowland areas (predicted wetlands and streams) and facultative upland species found predominantly in more well drained areas. This research contributes to the knowledge and understanding of the ecological requirements of bryophytes and how they are distributed across the landscape. Spatial information of this sort could be valuable for agencies involved in biodiversity conservation, restoration, or related management and regulatory efforts.

Effects of Sleep Restriction on Components of Attention

Jasmyn Cunningham (Dalhousie University)

Presented at the 39th Annual Science Atlantic Undergraduate Psychology Conference, May 18-19, 2015

Winner of the Karen Nicholson Award in Neuropsychology

It is well known that most people need, on average, eight hours of sleep per night. However, many people do not get this much daily sleep as a result of conflicting schedules, commitments, and other extraneous factors. Attention is a complex function that includes several separate, but interacting neural systems guiding vigilance (readiness to respond), orienting (searching for and the selection of stimuli for further processing) and executive control (attention resource allocation) abilities. It is not clear which of these underlying component processes of attention are most affected by sleep loss. The Dalhousie Computerized Attention Battery (DalCAB, 8 computerized reaction time tasks purported to measure aspects of vigilance, orienting and executive control) was administered on two occasions (within subjects design) to healthy participants (women aged 19-25 years), once after a nine hour overnight sleep opportunity and a second time after a three hour overnight sleep opportunity (sleep deprivation condition). Self-ratings of sleepiness and mood states were also obtained following each sleep condition. Interim results evaluating which attentional systems are affected by acute sleep loss will be reported.

Forensic Determination of Organic Substance Sources in the 1B Mine Pool of Sydney Coalfield Abandoned Mines

Ceilidh MacDonald (Cape Breton University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2105

Winner of the Analytical Chemistry Award, oral

Cape Breton has a long history of coal mining. The huge network of abandoned, flooded coal mines underground has proved to be an environmental issue for many years due to acid mine drainage and its impact on the surrounding environment. It has been suggested that organic materials are contaminating the mine water, and the aim of this work is to determine the source of the organic contaminants.

In this work, a GC-MS method was tested for the separation and detection of relatively polar compounds on a non-polar column. These compounds were analyzed using two non-polar columns, an NSP-PAH and an NSP-5 inert column. The NSP-PAH being slightly more polar but the NSP-5 having better separation and efficiency for this type of analysis. A method was also developed for UPLC-ESi-MS using both an isocratic system and a solvent gradient. The solvent gradient method did not produce any results and so it was not developed.

Water samples taken from seven sampling sites in the 1B mine pool area were analyzed using GC-MS, UPLC-ESi-MS and ICP-MS. Several organic compounds were tentatively identified through the NIST Spectral Search library with GC-MS. No conclusive evidence was found for the contamination of the 1B mine pool by organic compounds.

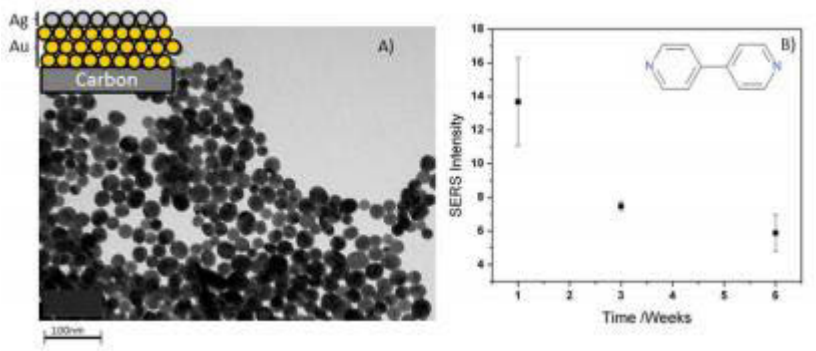
The Longevity of Modified Screen Printed Carbon Electrodes Using Surface-Enhanced Raman Spectroscopy

Jacquelyn White (Saint Mary's University)

Presented at the 40th Annual Science Atlantic / CIC Student Conference, May 21-23, 2105

Winner of the Analytical Chemistry Award, poster

Point-of-care (POC) diagnostics based on biosensing technology is of increasing interest for rapid disease diagnosis in limited resource settings. Such biosensors must exhibit long term stability such that year long shelf lives are possible. In 2013, screen printed carbon electrodes modified with layers of gold and silver showed promise as a platform in the detection of preeclampsia[1] . Current research aims to explore the shelf life of our SERS substrates. Screen printed carbon electrodes were modified with multiple layers of silver and/or gold nanoparticles. Using surface-enhanced Raman spectroscopy (SERS), multiple electrodes were tested to determine if the signal from two different indicator molecules, 4,4-bipyrdine and 12-mercaptododecanoic acid, decreased over time. Over the seven week period that the electrodes were monitored, the signal increased for only those modified with layers of silver nanoparticles and incubated in 4,4-bipyridine. The modified gold and silver electrodes incubated in 4,4-bipyridine did not result in an increase of signal; instead the signal decreased as expected. All those incubated in 12-mercaptododecaoic acid also had the resulting signal decrease as expected. Due to these mixed results, a repeat of Week 7 and on-going monitoring of the electrodes is required.



Figures: A) A TEM image of the silver nanoparticles present on the modified screen printed electrode. B) SERS intensity for the 1611cm^{-1} peak for 4, 4-bipyridine as a function of time.

[1] Zhao, L; Blackburn, J; Brosseau, C. Quantitative Detection of Uric Acid by Electrochemical-Surface Enhanced Raman Spectroscopy Using a Multilayered Au/Ag Substrate. *Anal. Chem.,* 2015, **87**, 441-447

HPLC Analysis of Various Photochemical Products Derived from Ru(II) Polypyridyl Complexes

Julia McCain (Acadia University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2105

Winner of the Biological/Medicinal Chemistry Award, poster

Photodynamic therapy (PDT) is a method for destroying unwanted cells, including cancer and bacteria. The process utilizes a photosensitizer (PS) that creates singlet oxygen from excited triplet states when exposed to light. While singlet oxygen is very effective at destroying cells, many cancer cells are hypoxic which limits the effectiveness of PDT for some of the most malignant and drug-resistant tumours. Therefore, our research group is exploring PSs that employ oxygen-independent mechanisms for light-triggered cell death. Generally, these PSs are strained Ru(II) coordination complexes that photoeject one bidentate ligand when activated with light. The resulting solvated species can then covalently modify DNA, a process that destroys cancer cells and tumours. High-pressure liquid chromatography (HPLC) is a convenient way to study these light-responsive agents as the unirradiated compounds, their photoejected bidentate ligands, and the solvated photoproducts are readily distinguished based on their unique retention times. My project involves characterizing these compounds and their photoproducts by HPLC in different solvents and under a variety of irradiation conditions. My poster will highlight some of these studies that feature strained Ru(II) complexes of 2,2'- biquinoline (biq) and substituted imidazo[4,5-*f*][1,10]1phenathrolines.

Development of a Bacterial Osmotolerance Complement Assay for methylthiohydroxybutyrate S-Methyltransferase Candidate Screening

Jessica Reiniger (Mount Allison University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2105

Winner of the Biological/Medicinal Chemistry Award, oral

Dimethylsulfoniopropionate (DMSP) is an abundant sulfur compound made by various algae, phytoplankton, and halophilic plants. Great environmental significance is attributed to both DMSP and its catabolite dimethylsulfide (DMS), in contributing to global sulfur cycling, cloud condensation and cooling. Furthermore, diverse physiological functions have been suggested for DMSP, focusing on stress adaptation, cryoprotection, hydroxyl radical scavenging, and osmoprotection. In particular both DMSP and dimethylsulfoniohydroxybutyrate (DMSHB) are classified as compatible osmolytes due to their zwitterionic structure and ability to equalize cellular volume under dehydrating conditions. DMSP biosynthesis in marine algae is a 4-step pathway with the third reaction catalyzed by an *S*-adenosyl-methionine-dependent *S*-methyltransferase that converts methylthiohydroxybutyrate (MTHB) to DMSHB. This is the first irreversible and therefore committing reaction in DMSP synthesis. To identify the gene encoding this methyltransferase, DMSHB's osmoprotectant ability was exploited. Using the *Escherichia coli* KEIO mutant collection and $P1_{vir}$ bacteriophage lysate transduction, a double mutant was constructed deficient in trehalose and glycine betaine compatible osmolytes. These mutations were confirmed by Sanger DNA sequencing. The osmosensitive strain was then used to define functional complementation assay conditions using osmotic stress. Addition of exogenous DMSP, while producing a negligible effect in unstressed conditions or with wild type strains, produced pronounced growth rate improvement in the mutant under salt stress.

Using the developed functional complementation assay, an existing *Ulva intestinalis* cDNA library was used to transform the osmosensitive *E. coli* mutant and screen for clones harbouring putative MTHB S-methyltransferase gene candidates. This system has been successful in producing growth phenotype differences and identified clones which are undergoing more detailed analysis.

Ruthenium Coordination Complexes with Pi-expansive Functional Ligands as Photosensitizers for Photodynamic Therapy

Leah Bennett (Acadia University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Inorganic Chemistry Award, poster

Photodynamic Therapy (PDT) is a non-invasive technique that combines a photosensitizer (PS) and light to kill cancerous cells. PDT involves administration of the PS to the patient, followed by a light treatment after the PS has localized in the tumour. Light activation of the PS produces an excited triplet state that can participate in Type II (energy transfer) and Type I (electron transfer) photoprocesses to create cytotoxic reactive oxygen species (ROS) only at the site of the tumour. While PDT is inherently selective, it is not effective against hypoxic tumours. The development of metallodrug PSs may be the solution to this issue. Metal-based PSs that can switch between oxygen-dependent and oxygen- independent cytotoxic mechanisms depending on tumour oxygenation status are being developed in our laboratory. One approach utilizes strained bis-heteroleptic Ru(II) coordination complexes that photoeject a bidendate ligand and covalently modify DNA, which halts replication and destroys the targeted cells. This light-triggered photoejection does not require oxygen. However, the Ru(II) complexes also incorporate an unstrained pi-expansive “functional” ligand that can sensitize ROS production when oxygen levels are sufficient. The expanded pi system of this ligand also provides a lipophilic handle for associating with biological macromolecules like DNA. My project involves combining the strained 2,2’-biquinoline (biq) ligand with various pi-expansive ligands in order to gain insight into the implications of extended pi-systems on the performance of bis- heteroleptic Ru(II) coordination complexes as photoejectors and as PSs. I will discuss the synthesis and characterization (^{1}H NMR, mass spectroscopy, and HPLC) of some of these compounds, and provide examples of their photobiological activities.

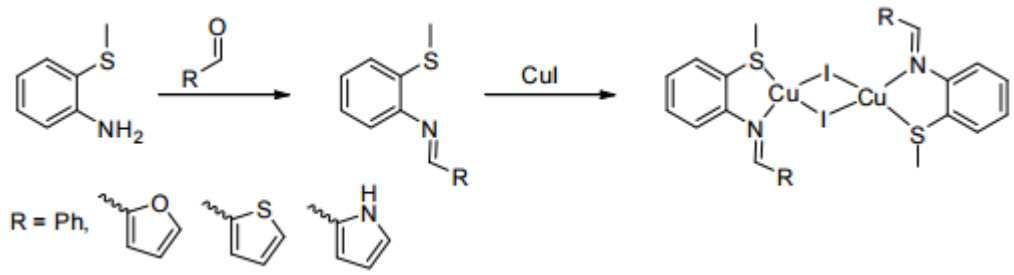
Synthesis of *N,S*-Ligands and Cu Complexation

Doug Richards (Cape Breton University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Inorganic Chemistry Award, oral

The development of new antibiotic drugs remains a necessity for public health. In our lab, we have synthesised a series of *N,S*-ligand systems based on the *ortho*-amino-thiophenol motif that can be complexed to Cu(I) and Cu(II). We modified the *N,S*-ligands with coordinating and non-coordinating pendants by Schiff-base reaction of the *ortho* (S-methyl) thioaniline with corresponding aldehydes in moderate to high yields. The pendants include phenyl, furan, thiophene and pyrrole groups. We obtained single X-ray crystallographic structure of the Cu(I) complex as a dimer with a Cu-$(I)_2$-Cu bridging motif. Some of these Cu complexes have been proven to show antibiotic effects when tested with selected strains of gram positive and gram negative bacteria.



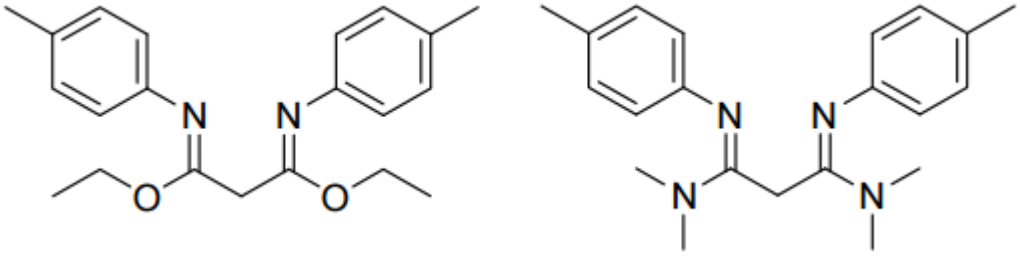
A New Class of Electon-Rich βDiketiminates

Bright Huo (Saint Mary's University)

Presented at the 40th Annual Scence Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Materials Chemistry Award, poster

The β-diketiminate family of ligands is used extensively in synthetic chemistry as both a way to stabilize reactive species and also as a framework to prepare molecules with high catalytic activity (Qian et al., 1998). Here we describe the preparation and reactivity of a new class of β-diketiminate ligand that possesses electron-donating groups on the ligand backbone. The synthesis of the modified β-diketiminate was performed and complexes have been prepared using the new ligand.



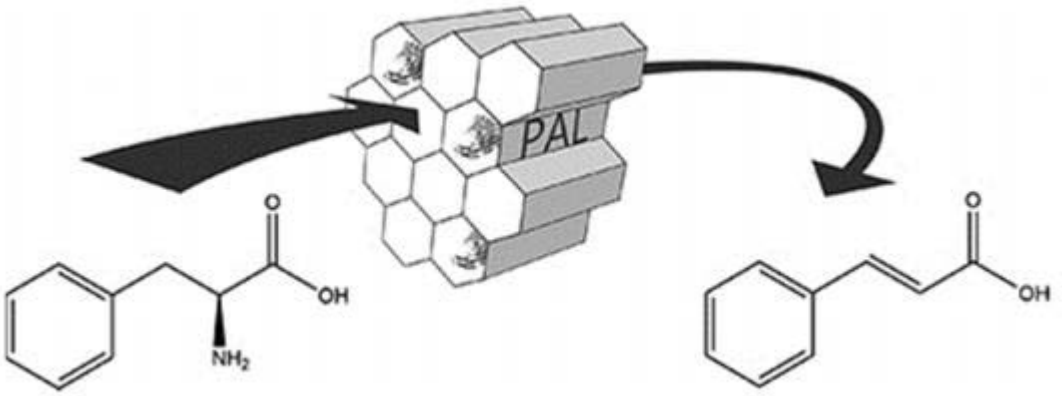
Entrapment of PAL in Mesoporous Materials

Matthew Tobin (Cape Breton University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Materials Chemistry Award, oral

Phenylalanine ammonia lyase (PAL), was entrapped in ultra-large-pore mesoporous silica (ULPS) (25 nm pore diameter) generating a recyclable, separable biocatalyst. The entrapped ULPS-PAL materials showed excellent stabilization, even after significant exposure to prolonged heating. Additionally, the entrapped ULPS-PAL materials showed extremely high catalytic activity in the deamination of L-phenylalanine to trans-cinnamic acid in aqueous solution and were recovered and recycled up to five times without any observable los- in activity. This approach is simple and capitalizes on the facile synthesis and easy recoverability of periodic mesoporous silicas to generate a stable, reusable PAL based biocatalyst.



Australian Journal of Chemistry 68(3) 396-400 http://dx.doi.org/10.1071/CH14603

A Twisted Look at the Synthesis of a Strained Isoindolinone

Jonathan Cann (University of New Brunswick, Fredericton)

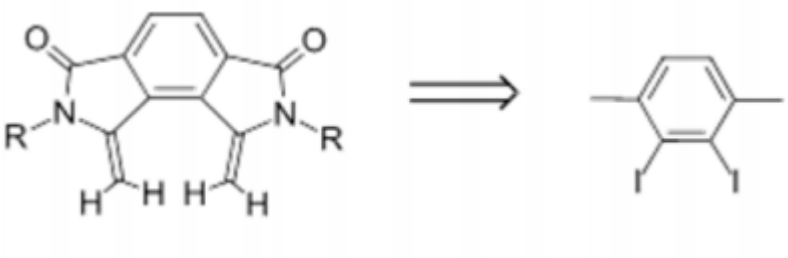
Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Organic Chemistry Award, oral

The ability to precisely control the physical and electronic properties of organic compounds is necessary for their ultimate applications in organic electronics, and responsive materials.[1,2] Our approach to the creation of organic materials is the design and synthesis of small monomer units for incorporation into oligomers and polymers. One way of modifying properties is to play with the planarity, which has been shown to have significant effects on electronic properties.[2] In the molecule below, due to the positioning of the 5-membered rings, the vinyl protons are placed in very close proximity. This feature is expected to twist the molecule, including the central benzene, out of planarity. We will explore the effect of the twisting on the stability, reactivity and electronic properties. The synthesis of this compound will also be discussed.

1. M. Lawson, S. Eisler. *Org & Biomol Chem*. **2012**, *10,* 8770-8773.

2. G. Bodwell, J. Bridson, M. Cyrañski, J. Kennedy, T. Krygowski, M. Mannion, D. Miller. *J. Org. Chem.* **2003** *68*, 2089-2098.



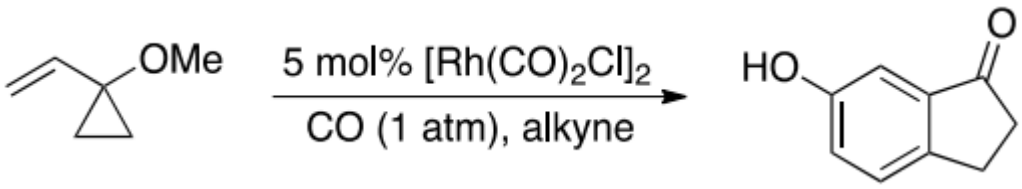
A Density Functional Theory Investigation of the Rhodium-Catalysed [5 + 1 + 2 + 1] Cycloaddition Reaction

Ifenna Mbaezue (Saint Mary's University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Organic Chemistry Award, poster

A [5 + 1 + 2 + 1] cycloaddition reaction is a rhodium-catalysed four-component reaction that leads to hydroxydihydroindenone products. This cycloaddition occurs only under a carbon-monoxide atmosphere; in the absence of CO, a [5 + 2] cycloaddition occurs yielding 7-membered carbocycles. We have employed density functional theory to elucidate the mechanism of this complex reaction system. Calculations were performed at the B3LYP/LANL2DZ level of theory. Results suggest that the reaction proceeds first through coordination of the vinylcyclopropane unit to the Rhodium catalyst, followed by C-C bond activation. Subsequently, a series of coordination and insertion processes occur to incorporate a CO molecule, an alkyne, and a second CO. Reductive elimination leads to an Rh-coordinated 9-membered carbocyclic intermediate. Decomplexation, 6π-electrocyclization, then elimination of MeOH lead to the final product.



Prediction of Stable Fe(III) Chlorine Species through an Ab Initio Study

Zoe Paula (Saint Mary's University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2105

Winner of the Physical, Theoretical, or Computational Chemistry Award, poster

As part of the Generation IV International Forum, CANDU and AECL are pursuing research into a Super Critical Water Reactor (SCWR). One of the main areas of study in this pursuit is the balancing and control of water chemistry within the nuclear reactor. The reactor will be run at approximately 650°C and 25 MPa, making experimental research difficult, and therefore the preliminary work is being done computationally. In this project complexes of iron (III), chloride and water where studied to find the most likely corrosion products by comparing the energy levels of the modeled complexes. The Unrestricted Hartree-Fock (UHF), second order Møller-Plesset (MP2) and Density Functional (B3LYP) levels of theory were used. Within each level of theory the basis sets 6-31G(d) and 6-31+G(d) were used. The complexes that fit $[Fe(Cl)_n(H_2O)_m]^{3-n}$ where $m+n \leq 6$ were looked at for this study as show in Figure 1.

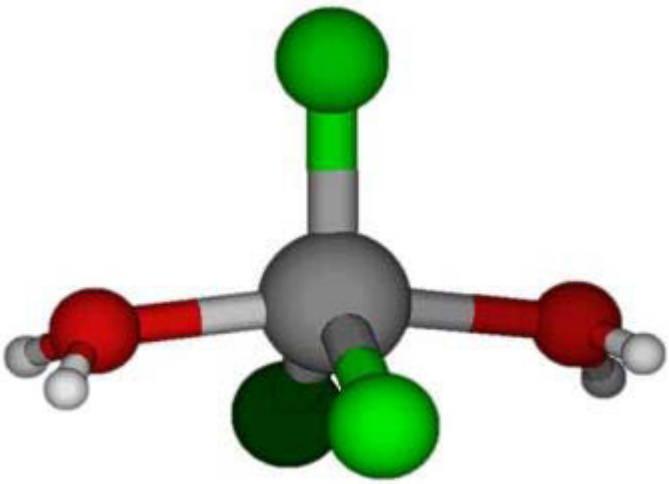


Figure 1: Model of $Fe(Cl)_3(H_20)_2$ found to be stable at C_2 symmetry have have total energy of -2797 Hartrees.

Photochemical Evaluation of Ruthenium-Based Photoejecting Coordination Complexes for Use as Photosensitizers in Photodynamic Therapy

Mitch Pinto (Acadia University)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Physical, Theoretical, or Computational Chemistry Award, oral

Photodynamic therapy (PDT) is a treatment that has been applied to various diseases with success, including several forms of cancer, osteomyelitis, and age-related macular degeneration. PDT is based on the idea that when a photosensitizer (PS) absorbs light, electronic redistribution produces an excited state that can take part in electron (Type I) or energy (Type II) transfer. However, other mechanisms for PS- mediated phototherapy are possible. When one or more ligands of a bis-heteroleptic Ru(II) complex causes steric clash within the complex, excited state photoejection of a ligand can occur. The product of this photoejection is capable of binding with DNA and killing targeted cells. Like Type I and Type II PDT, photoejection is spatially and temporally selective due to localized delivery of light to the targeted cells containing the PS. Treatment can be customized to specific cases by variation of PS, light dose/source/wavelength, and PS-to-light intervals. This presentation will discuss three ruthenium-based photoejectors, specifically [Ru(6,6'-dmb)2(ipt)]2+, where 6,6'- dmb=6,6'-dimethyl-2,2'-bipyridine and ipt=2-(2-thienyl)-imidazo[4,5- f][1,10] phenanthroline; [Ru(6,6'-dmb)2(ipbt)]2+, where ipbt=2-(2,2'-bithiophene)- imidazo[4,5- f][1,10] phenanthroline; and [Ru(6,6'-dmb)2(iptt)]2+, where iptt=2-(2' ,2'' :5'',2''' -terthiophene)-imidazo [4,5- f][1,10] phenanthroline. Structure-activity relationships will be discussed as a function of the number of thiophene units in the functional ligand by comparing photoejection plots, half-life values, and photobiological activities against bacteria and cancer.

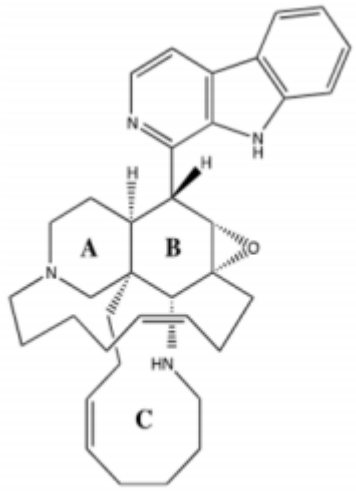
Synthesis of a model ABC-tricyclic Mmanzamine Core Using an Intramolecular Diels-Alder Approach

Jordan Donahue (University of New Brunswick, Fredericton)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

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

Throughout history, secondary metabolites (natural products) have provided a fundamental source of drugs for fighting infection, inflammation and cancer in humans. Of particular interest among these secondary metabolites is the manzamine family. In recent years, the manzamine alkaloids have been regarded as an interesting group of marine alkaloids with extraordinary biological activities, and as a result these molecules have received considerable attention for their chemistry and pharmacology. The diversity of biological activity for this class of compounds suggests that they may act on multiple targets, which could be controlled through synthetic modification. All of the manzamine alkaloids, except manzamine C, possess one of two general polycyclic skeletons. Manzamine A and its analogues possess a 6-6-5-8-13 polycyclic skeleton, whereas manzamine B and its analogues possess a 6-6-11-13 polycyclic skeleton. Currently, the MaGee group is working towards the synthesis of a tricyclic intermediate which will not only form the ABC-tricyclic core required for manzamine B and its analogues but also serve as a precursor which is adaptable for manzamine A and its analogues. The current approach involves synthesizing the macrocyclic C ring first and subsequently forming the AB ring system via an intramolecular Diels-Alder reaction, which has been found to proceed with high endo selectivity (25:1). Efforts to advance this key tricyclic intermediate towards our synthetic target will be communicated along with recent investigations into the utility of a domino Diels-Alder/ Intramolecular Schmidt reaction.



Manzamine B

High-Resolution Laser Spectroscopy of Ruthenium Monophosphide

Ricarda Konder (University of New Brunswick, Fredericton)

Presented at the 40th Annual Science Atlantic / CIC Student Chemistry Conference, May 21-23, 2015

Winner of the Murray Brooker Award in Chemical Education

This is the first known laser-spectroscopic analysis of ruthenium monophosphide (RuP), a linear diatom. Low-resolution analysis revealed two electronic transitions at 17,339.3 cm^{-1} (576.5 nm) and 16,893.23 cm^{-1} (591.8 nm) that were later confirmed to belong to RuP. Based on previous assignments of the ruthenium mononitride analogue by Ram et al, [1] it is hypothesized that RuP is associated with a $X^2\Sigma^+$ ground state. Dispersed fluorescence scans were performed of both bands and revealed the first six vibrational levels in the ground state. This allowed for the measurement of the approximate ground-state vibrational frequency of 515 ± 10 cm^{-1}.

High-resolution spectra were taken for both electronic transitions; from these, an initial estimate of the rotational constant and bond length for the main isotopologue (^{102}RuP) could be computed, namely 0.35cm^{-1} and 1.43Å, respectively.

[1] Ram, R.S., Bernath, P.F. Fourier Transform Emission Spectroscopy of the $F^2\Sigma^+$-$X^2\Sigma^+$ System of RuN. *Journal of Molecular Spectroscopy*. 2002; **213**:170-8.

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