

2013 Science Graduate Studies Day

Abstracts

May 23rd, 246 McDougall Hall & Schurman Market Square,
University of Prince Edward Island

Keynote speaker presentation:

- **Dr William Montelpare, Margaret and Wallace McCain Chair in Human Development and Health**
- **Preventing concussion and spinal cord injuries through skill based training**

The Play it Cool™ (PIC) Safe Hockey Program was designed to enhance ice hockey coaches' abilities to teach hockey skills with an emphasis on safety using a structured, facilitated, online curriculum. The program consists of three modules that focus on strong skating skills, on-ice awareness, and risk management from a prevention perspective. PIC was delivered to coaches of players age 9 to 15 years. In addition to the online curriculum, the coaches were asked to complete a series of questionnaires both at the beginning and end of their season. These questionnaires dealt with: the coaches' general background and experience, level of knowledge related to concussions, coach self-efficacy and readiness to change, as well as survey on general injury attitudes, and values related to risk, pain and injury in sport. Coaches were also provided the opportunity to dialogue about both the online curriculum and content of the surveys on the "Coach Discussion Board." Information from these sources was then analyzed to develop a series of open-ended questions that form the basis on a focus group discussion on topics related to coaching and the role of the coach in injury prevention, teaching and playing hockey with an emphasis on safety, and behaviours and values associated with hockey, the role of the hockey organization (e.g. either local or provincial) in injury prevention, and the implementation and evaluation of the program. Outcomes from both the quantitative and qualitative inquiry include the need for research-based injury prevention strategies (versus popular media/belief), the challenges associated with implementing multifaceted interventions, the formal arrangements/agreements among stakeholders responsible for injury prevention, the key role played by coaches in promoting injury prevention strategies, and the need for monitoring injuries and changes in knowledge, attitudes and behaviour.

Affiliation: Department of Applied Human Sciences

Oral presentations (alphabetical by main author):

ESC: Environmental Sciences

HUB: Human Biology

MMS: Molecular and Macromolecular Sciences

- **Catherine McNeil (MSc-ESC) & H. Carolyn Peach Brown**
- **Youth livelihood strategies and environmental decision-making in the humid forest zone of Cameroon**

Youth are an important group within forest communities of Central Africa but are often underrepresented within decision-making structures. This is particularly important given the context of REDD+ (Reducing Emissions from Deforestation and Forest Degradation) which will affect those who are dependent on forests as a source of livelihood. This research aimed to understand whether youth (aged 19 – 30) gain a large proportion of their livelihoods from the forest and if they are currently represented in local decision-making institutions that relate to forest governance. Surveys, interviews, and focus groups were conducted in six villages in the Eastern province of Cameroon. Despite changes in educational opportunities, youth continue to derive a large proportion of their livelihoods from forest resources. However, changes have been noted in the gender division of work. While youth remain underrepresented in formal village authorities and forest management committees, they play a large role in the development and functioning of other institutions.

Affiliation: Department of Biology & UPEI Environmental Studies Program

● **Beth Pearce (PhD-MMS) & Russ Kerr**

○ **Semi-synthesis of a biologically inspired library of natural product mimics, from the lipophilic marine natural product β -Gorgonene**

Inspired by ilimaquinone and other biologically active sesquiterpenes, we have transformed a highly lipophilic, non-drug-like, marine natural product (gorgonene), available as a by-product from the purification of pseudopterisins, into a library of more drug-like derivatives. Our strategy utilizes semi-synthesis to attach suitable structures such as substituted aromatics and heteroaromatics to the gorgonene scaffold to increase its drug-likeness and mimic natural product structures in biological systems. Several synthetic techniques are being explored to incorporate these interesting substructures in a minimum number of steps. The main focus of in this presentation will be an isoxazoline family of compounds resulting from a 2+3 cycloaddition reaction. The PTP1B (potential therapeutic target for treatment of type 2 diabetes) of the synthesized compounds will be discussed as well as some unexpected and interesting reactivity we have observed.

Affiliation: Department of Chemistry

● **Laura Phalen (MSc ESC)^a Bernd Köllner^b, Liane Leclair^a, Natacha Hogan^c, & Michael van den Heuvel^a**

○ **Immunotoxic effects of benzo[a]pyrene *in vivo* and *in vitro* in rainbow trout (*Oncorhynchus mykiss*)**

Polycyclic aromatic hydrocarbons (PAHs) are carcinogenic and immunotoxic. They are found virtually everywhere in the environment as they are produced by such events as forest fires and burning of carbon based fuels. Immune system studies in fishes are lacking, and yet these compounds are present in the aquatic environment, particularly in the oil sands development areas of northern Alberta, Canada. Our study looks at the effects of the prototypical PAH, benzo[a]pyrene (BaP), on the rainbow trout immune system. Intraperitoneal injection of BaP showed decreased immune cell counts in several tissues, and decreased circulating antibody produced in response to an antigen encounter. Follow up studies use *in vitro* techniques to begin to investigate the cellular level mechanism of this effect.

Affiliations: ^aDepartment of Biology & Canadian Rivers Institute, ^bFriedrich-Loeffler-Institut, Germany and ^cToxicology Centre, University of Saskatchewan, SK

● **Adam Proud (PhD-MMS) & Jason Pearson**

○ **An in depth analysis of bonding environments: Intracules and extracules**

There has always been a disconnect between many synthetic chemists and theoretical chemists. While synthetic chemists typically consider specific regions of a molecule to determine the reactivity, most of the work done by theoretical chemists is performed using canonical molecular orbitals (CMOs) which are delocalized over the entire molecule. However, localized molecular orbitals (LMOs) have been studied, albeit infrequently, for several years. These LMOs are far more chemically intuitive as they represent chemical bonds and lone pairs. The Pearson group has recently developed the localized pair model in which an electron pair within a bond, lone pair, or core orbital can be analyzed using various theoretical tools. One such tool is the extracule density which describes the distribution of the centre-of-mass of the electron pair with respect to the bond-midpoint. The results of said analyses will be discussed with a focus on the effects of electron withdrawing substituents on the extracule density.

Affiliation: Department of Chemistry

● **Christopher Rock (MSc-MMS), Alaa Abd-El-Aziz & Nola Etkin**

○ **The synthesis, characterization, and analysis of polynorbornenes containing various organometallic species**

Recently, our group has worked to incorporate new metals into polymers in order to determine their effects on the properties of the resulting materials. Initial work dealt strictly with iron containing polymers but has progressed to the inclusion of a second metal. This was initially done with the introduction of cobalt and, with this project, chromium. Incorporation of multiple metals was accomplished in two different ways. First, through the co-polymerization of a chromium containing norbornene with different iron containing norbornenes. This resulted in several new multimetallic polymers. Second, through the polymerization of a bimetallic iron-chromium norbornene. These compounds were then analyzed in order to assess their thermal properties

Affiliation: Department of Chemistry

● **Becca Striman (PhD-ESC), Donna Giberson & Christian Lacroix**

○ **Intraguild interactions and the limnological characteristics of the purple pitcher plant (*Sarracenia purpurea*): Potential applications for study**

Pitcher plants are an ideal experimental unit, as each pitcher can contain its own ecological community and vary in responses to the surrounding environment. The pitcher-shaped leaves of the plant capture rain water and attract insect prey, which provide nutrients not readily available in the bog. The leaves also provide a habitat for micro-organisms and at least three species of aquatic insect larvae (inquilines): the pitcher plant mosquito, midge, and flesh fly, which also feed on the captured prey in pitchers. Although much attention has been given to these insects, there is still controversy over the nature and importance of interactions among all players in this community. Even less is known about the water characteristics found inside the pitcher. The microlimnological characteristics of the pitcher habitats were studied in Glenfinnan Bog, Prince Edward Island and large diurnal and seasonal fluctuations in pH, conductivity, and dissolved oxygen were found. Of note, diurnal pH fluctuations were cyclic and appeared to relate to CO₂ variations from photosynthesis and respiration. Future experiments are planned to examine nutrient dynamics within the pitcher plant and pitcher habitat and the extent to which the interactions within the feeding guild (the pitcher plant and inquilines) and prey influence fitness in guild members.

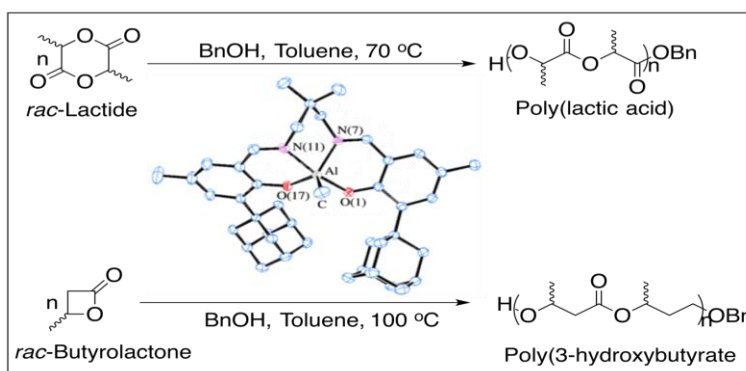
Affiliation: Department of Biology

Poster presentations (alphabetical by main author):

● **Christian Agatemor^a & Michael Shaver^{a,b}**

○ **Electronic Effects of Substituents on the Phenylene Backbone of Aluminium Salophen Complexes in the Ring-opening Polymerization of *rac*-Lactide and *rac*-β-Butyrolactone**

Three aluminum salophen complexes and an aluminum salen complex were synthesized and screened for stereoselectivity and polymerization rates of *rac*-lactide and *rac*-β-butyrolactone. All salophen complexes afforded atactic poly(lactic acid). Interestingly, the salophen complexes and the salen complex biased the microstructure of poly(3-hydroxybutyrate) towards syndiotacticity and isotacticity, respectively. Further, the salen complex was more active than the salophen complexes by a factor of 5 and 13 in the polymerization of *rac*-lactide and *rac*-β-butyrolactone, respectively. Last, a salophen complex with an electron-donating group on the backbone offered a faster polymerization reaction compared with a salophen initiator with an electron-withdrawing group.



Affiliation: ^aDepartment of Chemistry and ^bSchool of Chemistry, University of Edinburgh, UK

● **Alberto, Ashley, Michael van den Heuvel & André St-Hilaire**

○ **Monitoring stream sediment loading and biological responses on Prince Edward Island**

PEI is known for its sedimentation problems due to intense agricultural land-use. In addition to the mandated riparian buffer zones, programs such as the Alternative Land Use Service program have been implemented to

minimize the impacts of these activities by encouraging better land management practices. However, there is no known historical data quantifying sediment loading and there is currently no way to assess the success of these programs. The first aim of this study is to examine the impacts of agriculture on sedimentation on PEI and develop a cost effective methodology for ongoing monitoring. Sedimentation on PEI has been of particular concern because of its potential to impact salmonid spawning habitat. In fact, Atlantic salmon is present in only a fraction of its former range on PEI. The second part of this study will serve to assess the effects of sedimentation on fish reproductive habitat by examining the emergence and survival of salmonid eggs *in situ*. The outcome of the study will be the establishment of a monitoring framework for sediments and their biological effects on PEI. The study data will provide a baseline to the province with which to evaluate subsequent change, and to establish sediment loading targets in the watershed. The novel aspect of this study makes it of great importance to the province of PEI as well as to the greater scientific community.

Affiliation: Department of Biology and Canadian Rivers Institute

● **Brittany Cole, Jamie Butler & Karen Samis**

○ **Adaptation to the ecological limits in a coastal habitat**

Every species has an ecological limit, but not all species are capable of evolving and expanding beyond that limit. Habitat margins are of particular interest to ecologists since they may represent limits in the ability to survive and adapt to an environmental change. The annual plant, *Cakile edentula*, is one of few plants endemic to the ecological gradient stretching from open sandy beach to densely vegetated dunes. Empirical and experimental research in our lab shows that *C. edentula* has higher fitness growing on the beach than in the dune. The purpose of my research is to assess the ecological limits of *C. edentula*, and the ability of the plant to adapt to or beyond its current limits in the ecologically marginal beach habitat. This summer, I will conduct a field transplant experiment in PEI and NS to test whether phenological differences in wild populations are due to plastic responses to habitat or genetic variation between beach and dune. Demographic surveys will be continued to quantify the abundance of *C. edentula* populations on several maritime beaches. Taken together, these data will provide a description of the demographic and ecological correlates of fitness in this species. This research is significant to the understanding of ecological limits; and is important since we may predict that the implications of habitat change may be greatest at range margins

Affiliation: Department of Biology

● **Michael Coffin (PhD-ESC)^a, Michael van den Heuvel^a & Simon Courtenay^{a,b}**

○ **Assessing the effect of trophic cascades on eutrophication in estuaries of the southern Gulf of St. Lawrence**

Estuaries are important habitat for juvenile fish, important economically for fisheries (finfish and shellfish) and provide valuable ecosystem services. Seagrass is generally considered an indicator of estuarine health but is in decline worldwide, including the Southern Gulf of St. Lawrence. Inputs of limiting nutrients can lead to an increase of macroalgae, which displaces eelgrass and is inferior habitat for fish. Furthermore, when macroalgae are at high densities hypoxic or anoxic conditions can develop which can alter community composition and functioning. Alternatively, or concomitantly, the removal of top predators through over-fishing may have cascading effects on the community reducing its resilience to increased nutrient loads. Predicting hypoxia/anoxia requires an understanding of the relationship between the biotic community and abiotic variables. I intensively monitored water quality, using dissolved oxygen as the response variable, and investigated epifaunal distribution and density throughout five island estuaries. Preliminary results identified parameters that increase the likelihood of hypoxia/anoxia and highlighted knowledge gaps, which will be explored through focused field and laboratory experiments. Additionally, results from this study will be used to develop a monitoring framework for estuaries in the region.

Affiliation: ^aDepartment of Biology & Canadian Rivers Institute, ^bDepartment of Fisheries and Oceans

● **Krista Gill & Russ Kerr**

○ **Discovery of a novel peptide natural product from *Streptomyces* sp. RKKD-790**

Streptomyces sp. RKKD-790 produces a novel peptide natural product that is a member of the class II lasso peptides. It consists of 15 amino acids and contains a macrolactam ring formed between glycine at the N-

terminus and aspartic acid at the eighth amino acid position. The lasso fold is formed by the C-terminal tail irreversibly threading through a macrolactam ring and is held in place by Trp-14 and Leu-15 which act as bulky steric locks that prevent the linear tail from unthreading. It was discovered by analyzing LCMS profiles of a library of bacterial fermentation extracts using the multivariate statistic tool Principal Component Analysis. The structure was elucidated using NMR spectroscopy and the lasso fold was determined using tandem mass spectrometry and computational modeling from NOE distance constraints

Affiliation: Department of Chemistry

● **Alaa Abd-El-Aziz, Inan Kucukkaya (PhD-MMS), Mosa Alsehli & Brian Wagner**

○ **Synthesis and photophysical properties of novel porphyrin dendrimers and polymers containing organoiron complexes**

Porphyrin polymers, dendritic porphyrins and metalloporphyrins are of great interest for their applications in many fields such as light-energy conversion, photodynamic therapy (PDT), third-order non-linear optical materials, organic light-emitting diode (OLED) devices, fluorescence switches, and molecular wires. The synthesis and preliminary photophysical properties of novel porphyrin and metalloporphyrin dendrimers containing cationic η^6 -chloroarene- η^5 -cyclopentadienyliron(II) complexes functionalized with naphthalene and capped with ferrocene and condensation polymerization of disubstituted porphyrins with cationic η^6 -chloroarene- η^5 -cyclopentadienyliron(II) complexes are described. Linear polyether porphyrin polymers can be a great interest in purification of water from heavy metals. The incorporation of cationic η^6 -chloroarene- η^5 -cyclopentadienyliron moieties can enhance solubility and facilitate nucleophilic aromatic substitution, addition and condensation reactions due to the intense electron-withdrawing ability of the iron center. Divergent approaches were employed to give highly symmetrical branched materials. The preparation of these dendrimers was achieved via metal-mediated nucleophilic aromatic substitutions and Steglich esterifications. Porphyrin polymers, dendrimers and their precursors were characterized through nuclear magnetic resonance spectroscopy, infrared spectroscopy, ultraviolet-visible and fluorescence spectroscopy

Affiliation: Department of Chemistry

● **Hailey Lambe (MSc-ESC)^a, Marina Silva-Opps^a, Sheldon Opps^b, Will Robbins^a, Chuck Gallison^c & Brad Potter^c**

○ **Assessing home range and habitat selection of red foxes in Charlottetown, PEI: Project Design**

The red fox (*Vulpes vulpes*) is the second largest carnivore on Prince Edward Island and occupies most habitat types across the province including urban areas. Although very little information exists regarding the interactions of foxes and other canids, it has been suggested that in Prince Edward Island, the presence and pressures of coyote (*Canis latrans*) populations have displaced red foxes from rural settings to urban areas. Medium-sized carnivores, such as the red fox are considered “ideal” urban dwellers, as they exhibit a high level of plasticity in terms of diet, movement patterns and social behaviours. There remains to be many population attributes that are unknown for urban foxes. Learning more about this species will facilitate a better understanding of how the fox uses urban areas, and thus allow for appropriate management programs to be implemented in order to promote healthy animal-human interactions. The main goal of our study is to gather information on movement, habitat and den-site selection. We are proposing to use: sighting reports generated by the public, den surveys and information gathered by GPS collars to assess movement patterns, home range size and core area use as well as habitat selection of red foxes in Charlottetown.

Affiliation: ^aDepartment of Biology, ^bDepartment of Physics and ^cPEI Department of Environment, Energy & Forestry

● **Liane Leclair^a, Gillian MacDonald^a, Laura Phalen^a, Bernd Köllner^b, Natacha Hogan^c & Michael van den Heuvel^a**

○ **The Immunological effects of oil sands surface waters and Naphthenic Acids on rainbow trout (*Oncorhynchus mykiss*)**

There is concern surrounding the immunotoxic potential of naphthenic acids (NAs), a major organic constituent in waters influenced by oil sands contamination. To assess the immunological response to NAs, rainbow trout (*Oncorhynchus mykiss*) waterborne exposures were conducted with oil sands-influenced waters, NAs extracted

and purified from oil sands tailings waters, and benzo[a]pyrene (BaP) as a positive control. After a 7 d exposure, blood, spleen, head kidney, and gill samples were removed from a subset of fish in order to evaluate the distribution of thrombocytes, B-lymphocytes, myeloid cells, and T-lymphocytes using fluorescent antibodies specific for those cell types coupled with flow cytometry. The remaining trout in each experimental tank were injected with inactivated *Aeromonas salmonicida* and held in laboratory water for 21 d and subjected to similar lymphatic cell evaluation in addition to evaluation of antibody production. Fluorescent metabolites in bile as well as liver CYP1A induction were also determined after the 7 and 21 d exposure. Oil sands waters and extracted NAs exposures resulted in an increase in bile fluorescence at phenanthrene wavelengths, though liver CYP1A was not induced in those treatments as it was with the BaP positive control. Trout in the oil sands-influenced water exposure showed a decrease in B- and T-lymphocytes in blood as well as B-lymphocytes and myeloid cells in spleen and an increase in B-lymphocytes in head kidney. The extracted NAs exposure showed a decrease in thrombocytes in spleen at 8 mg/L and an increase in T-lymphocytes at 1 mg/L in head kidney after 7 d. There was a significant decrease in antibody production against *A. salmonicida* in both oil sands-influenced water exposures. Because Oil sands-influenced waters affected multiple immune parameters, while extracted NAs impacts were limited, the NAs tested here are likely not the cause of immunotoxicity found in the oil sands-influenced water.

Affiliations: ^aDepartment of Biology & Canadian Rivers Institute, ^bFriedrich-Loeffler-Institut, Germany and ^cToxicology Centre, University of Saskatchewan, SK

● **Gillian MacDonald & Michael van den Heuvel**

○ **Recovery of stickleback populations previously exposed to pulp mill effluent**

Fish exposed to pulp mill effluent are subject to a variety effects, mostly related to reproduction. With the use of e-documents becoming more and more popular, pulp and paper mills are becoming less relevant and thus shutting down. It is of interest to look at the recovery rates of fish once exposed to their effluent. This project looked at fish in an effluent receiving area of a once operational mill and compared them to fish in nearby reference sites. Parameters investigated included temperature, reproductive maturity, and CYP1A induction. Temperature was measured via tidbit loggers installed at sites, reproductive maturity was measured through histological staining, and CYP1A induction was measured through ethoxyresorufin-o-deethylase (EROD) analysis. Results indicated that during operational periods, temperature at the receiving area was consistently at least 3 °C warmer than reference sites. Reproductive maturity of the receiving area fish was generally higher than other reference sites, except for one. Receiving area fish had higher CYP1A induction compared to those at reference sites. Drawing clear and concise conclusions from these results is difficult as this project was initially developed under the impression that a closed mill would remain closed. The mill did not remain closed so many questions regarding recovery are now invalid. Currently, we plan to verify CYP1A induction with genetic analysis and investigate the possibility of sediment contamination and its role in CYP1A induction.

Affiliation: Department of Biology & Canadian Rivers Institute

● **Teri McComber, Jennifer Taylor, William Montelpare & Carolanne Nelson**

○ **Food group composition of elementary school children's lunches: changes in food group intakes associated with the implementation of school nutrition policies**

Schools across North America are implementing school nutrition policies (SNP) as a practical means of improving children's dietary intakes, particularly the foods consumed at school. In Prince Edward Island, SNPs have been implemented in all elementary schools since 2006, allowing for the assessment of changes over time in the dietary quality of children's school lunches and whether diet quality is associated with the SNP implementation. Although there is evidence regarding the impact of SNPs on children's nutrient intakes, we know little about the impact on children's lunch time food group intakes. The purpose of this study was (a) to describe school children's lunch time food group intakes in 2007 (early SNP implementation), 2010 (4 years after implementation) and 2012 (6 years after implementation) (b) To assess changes in intakes of Canada's Food Guide (CFG) from 2007 to 2012 and (c) To assess the relationship between the length of policy implementation, level of SNP adherence and children's lunchtime CFG and sub-grouping food group intakes. A validated lunch time food record was used to assess one day lunchtime intakes of grade 5 and 6 students in 2007

(n=1980), in 2010 (n=1642) and 2012 (n=1564). The proportion of children consuming adequate intakes of Vegetables and Fruits (VF) and Milk and Alternatives (MA) at lunch was low, with a higher percentage of students having Grain Products (GP) and Meat and Alternatives (MEA) intakes which meet one third of the daily CFG recommendations. Mean servings of the Low Fat Whole Grain Group ($p < 0.0001$) and the High Fat Whole Grain Group ($p = 0.0004$) both increased significantly over time. VF and MA did not increase over SNP implementation, which may be explained by the low availability of such foods in both home and school sources. Results indicate that, when followed, elementary school nutrition policies can have a positive, albeit modest impact on the quality of children's food intakes at school, particularly for the intake of whole grains. It is important to increase school adherence to SNPs and consider the source of foods consumed in order to investigate potentially positive impacts of the policy

Affiliation: Department of Applied Human Sciences

● **Luke McDougall & Robert Hurta**

○ **Magnolol affects expression of cell adhesion molecules in human prostate cancer cells**

Magnolol is a phenolic compound procured from the bark and roots of magnolia, *Magnolia officinalis*. Magnolol has been shown to have anti-cancer effects on *in vitro* treatments of human prostate cancer cells. The mechanisms by which magnolol exerts its anti-cancer effects are not well understood. Our hypothesis is that magnolol can affect the behavior of prostate cancer cells *in vitro* and these effects will include magnolol mediated changes in the migration, invasion and adhesion of prostate cancer cells. In this regard, preliminary findings suggest that in response to magnolol (40 μ M and 80 μ M) for 3, 6, and 24 hours, a decrease in I-CAM and in V-CAM protein expression levels (determined by Western blot analysis) occurred in DU145 human prostate cancer cells. These results suggest that magnolol mediated decreases in these adhesion-regulating proteins may contribute to decreases in DU145 cell adhesion. Studies are ongoing to further characterize these magnolol-mediated changes in DU145 cellular behavior (funded by the Jeanne and J.-Louis Levesque Foundation)

Affiliation: Department of Biology

● **Brendan McKeown^a, Catherine Neto^b & Robert Hurta^a**

○ **American cranberry (*Vaccinium macrocarpon*) extract affects insulin-like growth factor binding proteins in human prostate cancer cell lines *in vitro***

American cranberry (*Vaccinium macrocarpon*) extract has previously been shown to affect cell cycle, apoptosis and proliferative ability in cancer cell lines *in vitro*, particularly in prostate cancer cell lines. The insulin-like growth factors (IGFs) and their modulators, specifically the insulin-like growth factor binding proteins (IGFBPs) may play roles in these events. The IGFBPs act by regulating IGF action but also exhibit a range of IGF-independent activities. IGFBP expression in the DU145 and PC3 prostate cancer cell lines has been determined using Western blot analysis to show that protein expression levels of IGFBP-2 and IGFBP-5 decrease, IGFBP-4 increases and IGFBP-3 shows no significant change after exposure to whole cranberry extract (WCE). Prostate cancer cells progressing from androgen sensitivity to androgen independence express increased levels of IGFBP-2 and IGFBP-5, suggesting that WCE may play some role in counteracting this process *in vitro*. The changes in IGFBP expression observed in this study also indicate decreased IGF activity, suggesting an inhibition of cellular growth through this pathway. These WCE mediated changes in IGFBP expression are novel and further indicate the potential chemoprotective and chemopreventative actions of cranberry extract *in vitro*. This project is funded by the Cranberry Institute (Wisconsin Board) and the Jeanne and J.-Louis Lévesque Foundation.

Affiliations: ^aDepartment of Biology and ^bDepartment of Chemistry & Biochemistry, U Mass Dartmouth, USA

● **Brendan Sheppard & Jason Pearson**

○ **Electron-electron interactions from correlated to non-correlated methods. An intracule story**

Hartree-Fock (HF) theory is one of the earliest methods used by computational chemists to calculate the energy or properties of a chemical system. HF can be accurate, however it fails to properly account for electron correlation. Density functional theory is a fundamentally different method than HF, which is computationally cheap to use and it accounts for electron correlation. Previous work in our lab developed a new technique to analyze the distribution of electrons in chemical bonds and lone pairs using probability distributions of electron pairs, or intracules. This previous work however used the non-correlated HF method so it is important to

examine the effect correlation has on these intracules. This is an ongoing study but it has been noted that correlation increases inter-electronic separation, as expected, and that electron correlation may be less important in less electronegative bonds as observed by the differences in the intracules.

Affiliation: Department of Chemistry

● **Shiv Singh ver^a, Rabin Bissessur^b & William Whelan^a**

○ **Gold nanocages: How stable are they to be used as contrast agents in photoacoustic imaging to detect cancer**

Optoacoustic (OA) imaging is a new technique for cancer detection and non-invasive monitoring of cancer therapeutics. This technique is the combination of both optical and ultrasound imaging, in which tissue is irradiated with nanosecond laser pulses. The delivered optical energy is absorbed and converted into heat, leading to thermoelastic expansion which produces acoustic waves. Generated sound waves are then detected by ultrasonic transducers to form an image. In order to enhance optoacoustic signals in tissues, gold nanocages (AuNCs) can be used as contrast agents due to their tuneable optical properties in the near infrared region. Gold nanoparticles are biocompatible and their surface chemistry is well known, therefore they can be easily functionalized to target specific cells. This work involves an initial study to test the stability of AuNCs irradiated by laser pulses. The optoacoustic system consists of a Nd:YAG pumped Ti:S laser, which can operate at either 775 nm or 1064 nm, an 8 element annular array transducer with 5 MHz central frequency and bifurcated optic fibre bundles to introduce light to the target. A 6 ns pulse duration and 10 Hz repetition rate were used. Different pulse energies (5.3 mJ, 12.5 mJ, 21.6 mJ) were used and at each energy, three different AuNCs sample were exposed for 1 min, 3 min and 5 min. Optoacoustic and absorption spectroscopy techniques and transmission electron microscopy (TEM) imaging were used to analyze the AuNCs samples following laser exposure. The integrated optoacoustic signal obtained from AuNCs samples at the start and end of illumination showed a 33% decrease. Optical absorption data also showed a 20 nm blue shift and 12% decrease in peak amplitude. TEM images, before and after the irradiation confirmed the melting and fragmentation of AuNCs for a pulse energy of 21.6 mJ and an exposure of 5 minutes. This study confirms that structural changes in AuNCs can occur, leading to changes in their desired properties as contrast agents.

Affiliation: ^aDepartment of Physics and ^bDepartment of Chemistry



**Science Graduate Studies Committee
2013**