McMaster University

Inspiring Innovation and Discovery

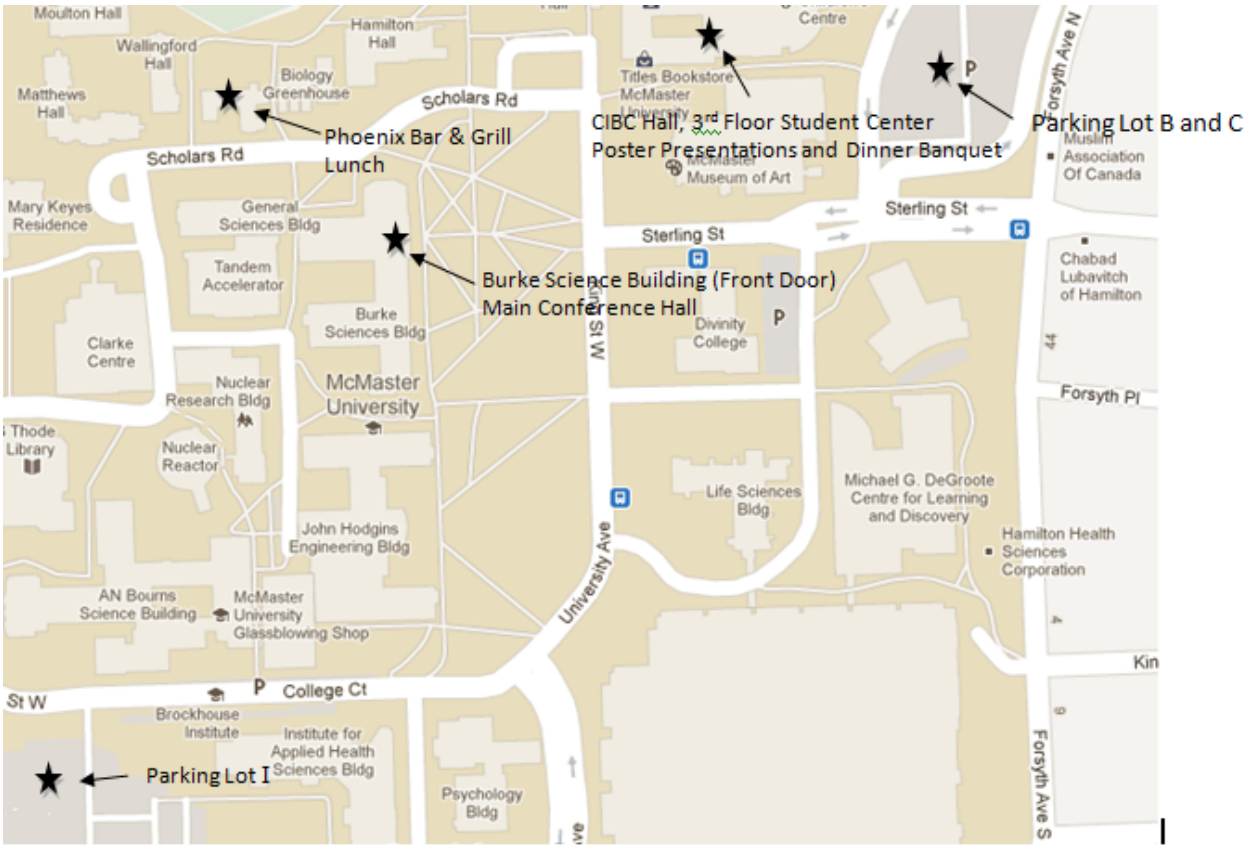
SOUSCC 2013

41st Southern Ontario Undergraduate Student Chemistry Conference

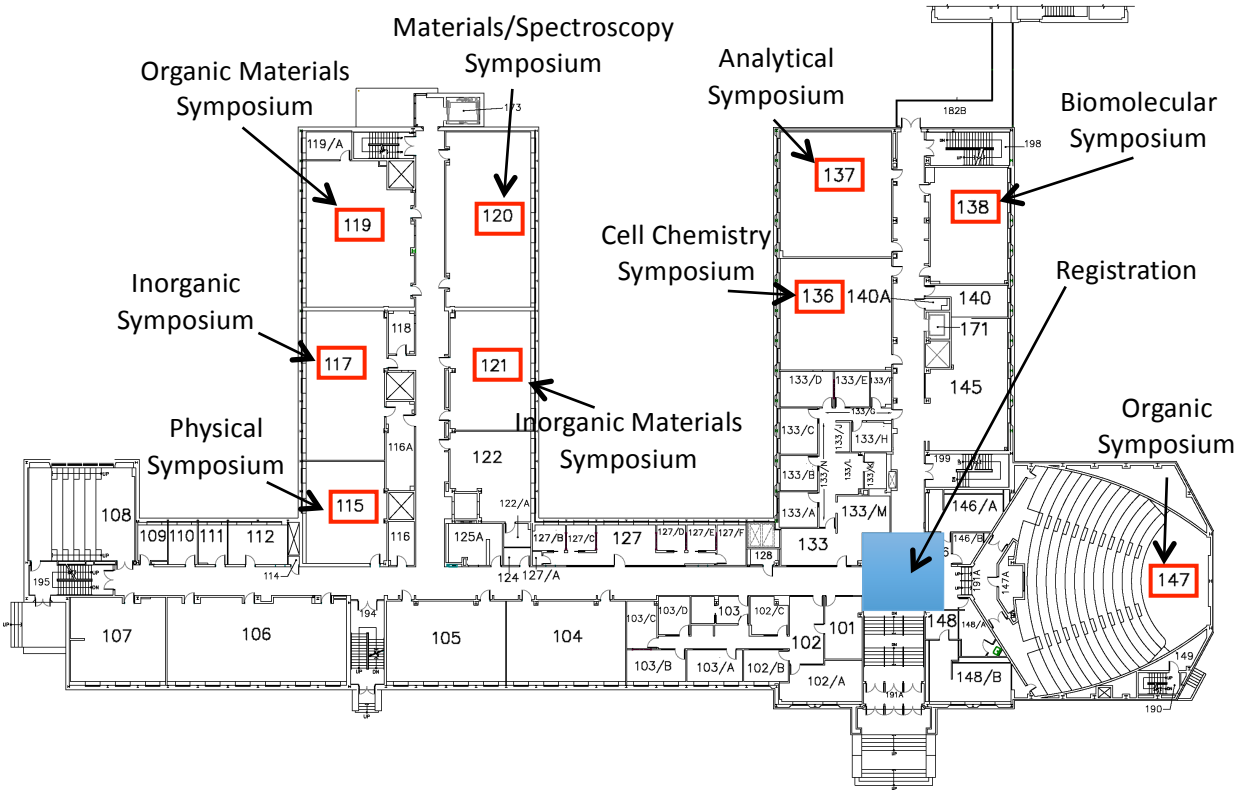
March 30th, 2013

MAPS

McMaster Campus



Burke Science Building



McMaster University

Department of Chemistry
and Chemical Biology

Dear SOUSCC Participant,

We are very happy to welcome you to the 41st annual Southern Ontario Undergraduate Student Chemistry Conference (SOUSCC), hosted by the Department of Chemistry and Chemical Biology at McMaster University. McMaster University is committed to the support of outstanding undergraduate and graduate research, and is a leader in innovative approaches to undergraduate education. We are particularly pleased to be hosting this conference again, as it epitomizes the values and ideals we hold for the training and education of undergraduates at McMaster, in Ontario and across Canada. The sharing of experimental results with professional peers is one of the cornerstones of modern research. It is a valuable exercise that leads to a rich professional career based on the collective creation and sharing of knowledge. It helps generate new ideas, broadens one's understanding of science, and initiates collaborations between like-minded individuals. The organizing committee has worked extremely hard to ensure that you have an enjoyable, educational, and memorable experience over the course of this day. Regardless of whether this represents your first conference, or one of many you have attended, we hope that you will learn from your peers, develop new friendships, and spark your interest in a lifelong career of chemical research.

This year we have 162 submitted abstracts including 135 oral and 27 poster presentations, which makes this is the largest SOUSCC ever organized and clearly indicates the broad interest in continuing the tradition of this event. We are particularly pleased to offer an expanded poster session that everyone can enjoy at the end of the day, once all the oral presentations are completed. We hope you will attend a number of sessions, learn about the exciting research being presented, and interact with colleagues. The ability to meet people from other institutions and discuss ideas with them is an important part of any conference, so please take the opportunity to interact with the large number of other students in attendance from across the province.

SOUSCC could not be successful without the generous support of numerous organizations. We thank all of our sponsors who value and support this conference, including the McMaster Faculty of Science, the McMaster School of Graduate Studies, the McMaster Academic Science Fund, and the Department of Chemistry and Chemical Biology. In addition, the c-IDEM CREATE program, the Chemical Institute of Canada, and the various divisions (listed at the back of this booklet) provided important funding toward this conference, and we could not have organized such a large meeting without their help. We would like to thank O'Zone Software for providing the Hermes abstract submission software, as well as VWR, Nelson Publishers, and Wiley for their generous donations. We would like to thank all the volunteers, judges, and session chairs that have generously given their time to help make this event a success. Finally we would like to thank you for your time and effort in contributing to this important annual undergraduate event.

We wish you the best of luck throughout the day, and a bright and prosperous future career in chemistry.

Sincerely,

Dr. Alex Adronov, Chair, SOUSCC41 Organizing Committee

SOUSCC COMMITTEE

Faculty Advisors

Dr. Alex Adronov (Conference Chair)
Dr Philip Britz-McKibbin
Dr. James McNulty
Dr. Jose Moran-Mirabal
Dr. Ignacio Vargas-Baca

Student Organizers

Tara Dickie
Nora Labbancz
Fahim Naeem
Faisal Adam Pany

LIST OF JUDGES

We would like to thank the following individuals for taking the time to assist with the judging of the poster and oral presentations:

Greg Bahun
Phil Britz-McKibbin
David Brock
Styliani Constas
Emily Cranston
Andy Dicks
Randy Dumont
Heather Gordon
Gillian Goward
Kris Harris
Richard Lee
Jim McNulty
Paul Piunno
Adam Ptolemy
Rob Schurko
Liliana Trevani
Dragan Vuckovic
Nathan Magarvey

SPECIAL THANKS

Volunteers

Dinesh Basker
Ryan Chadwick
Nicole DeAlmeida
Laura Dodge
Ian Duffy
Chris Gendy
Farnaz Heidarzadeh
Madiha Khan
Lana Kostina
Lucia Lee
Talena Rambarran
Nicole Rice
Lukas Sadowski
Leigh Spencer
Peng Wang
Nadine Wellington
Carlos Zepeda Velazquez
Yujie Zhu

McMaster Undergraduate Society for the Chemical Sciences
Housing and Conference Services
Paradise Catering

PROGRAM

TIME	ACTIVITY	LOCATION
8:00 – 9:00 A.M.	Registration/Continental Breakfast	Lobby BSB
9:00 – 9:30 A.M.	Plenary Session: "Improving Your Image - The Chemistry of Molecular Imaging" by Dr. John Valliant, Associate Professor; Scientific Director and CEO of the Centre for Probe Development and Commercialization	BSB – 147
9:40 – 10:40 A.M.	Oral Presentation Symposia	BSB Rooms
10:40 – 11:00 A.M.	Coffee Break	Lobby BSB
11:00 A.M. – 12:20 PM	Oral Presentation Symposia	BSB Rooms
12:20 – 1:40 P.M.	Lunch at the Phoenix Bar and Grill	Phoenix
1:40 – 3:00 P.M.	Oral Presentation Symposia	BSB Rooms
3:00 – 3:20 P.M.	Coffee Break	Lobby BSB
3:20 – 5:00 P.M.	Oral Presentation Symposia	BSB Rooms
5:30 – 6:30 P.M.	Poster Session/Mixer	CIBC Hall
6:30 – 9:30 P.M.	Banquet and Awards Ceremony	CIBC Hall

Improving Your Image - The Chemistry of Molecular Imaging Dr. John Valliant, Ph.D.

We are delighted to have Dr. John Valliant deliver the plenary lecture for our conference. Dr. Valliant pursued his doctoral studies at McMaster University and subsequently completed his post-doctoral training under the guidance of Profs. Alun G. Jones (Harvard University) and Alan Davison (Massachusetts Institute of Technology). Dr. Valliant became a faculty member at the Department of Chemistry and Chemical Biology at McMaster University in 1999.

Currently, he serves the department as an Associate Professor, specializing in radiopharmaceutical chemistry in addition to serving as the Scientific Director and CEO of the Centre for Probe Development and Commercialization (CPDC). The CPDC is focused on the development and commercialization of imaging probes and technologies to combat shortages of medical isotopes in Ontario and across Canada. Dr. Valliant has had a vibrant career so far with numerous publications and several patents in the area of radiopharmaceuticals and imaging probe development.

Symposia Timetable

TIME/ROOM	BSB – 147	BSB – 115	BSB – 117	BSB - 119	BSB – 120	BSB – 121	BSB – 136	BSB – 137	BSB – 138
8:00 – 9:00 A.M.	Registration – Continental Breakfast – BSB Lobby								
9:00 – 9:30 A.M.	Plenary Session								
9:40 – 10:40 A.M.	Organic	Physical	Inorganic	Organic Materials	Materials – Spectroscopy	Inorganic Materials	Cell Chemistry	Analytical	Biomolecular
10:40 – 11:00 A.M.	Coffee Break								
11:00 A.M. – 12:20 PM	Organic	Physical	Inorganic	Organic Materials	Materials – Spectroscopy	Inorganic Materials	Cell Chemistry	Analytical	Biomolecular
12:20 – 1:40 P.M.	Lunch – Phoenix Bar and Grill								
1:40 – 3:00 P.M.	Organic	Physical	Inorganic	Organic Materials	Materials – Spectroscopy	Inorganic Materials	Cell Chemistry	Analytical	Biomolecular
3:00 – 3:20 P.M.	Coffee Break								
3:20 – 5:00 P.M.	Organic	Physical	Inorganic	Organic Materials	Materials – Spectroscopy	Inorganic Materials	Cell Chemistry	Analytical	Biomolecular
5:30 – 6:30 P.M.	Poster Session – CIBC Hall								
6:30 – 9:30 P.M.	Banquet and Awards Ceremony – CIBC Hall								

Saturday AM

BSB Foyer

2013 SOUSCC

08:00 Registration and continental breakfast

Continues until noon.

Plenary Lecture BSB147

09:00 Improving your Image - The Chemistry of Molecular Imaging John F. Valliant

Organic BSB-147

Chair: Ryan Chadwick

09:40 0007 *Synthesis of novel 1,2-dihydropyridazine-3,6-dione derivatives of 1,3,5-sym-traizine and screening for their antimicrobial activity* **Thakkar M**, Mikhaylichenko L

10:00 0039 *Designing and Synthesizing Bimodal, Di-Salicylic Acid PTP Inhibitors* Gunning P.T, Haftchenary S.H, Ball D.B, **Jouk A.J**

10:20 0167 *Structure determination and application of peptide macrocycles from aziridine aldehydes* **Ler S**, Zaretsky S, White C, Scully C, Yudin A

10:40 Coffee Break

11:00 0076 *Parallel synthesis of a diverse library of pyridinone based compounds to probe the chemical space of binding to L-glutamine: D-fructose-6-phosphate Amidotransferase (GFAT)* **Bagha B.S.**, Walter L.A., Capretta A.

11:20 0035 *Synthesis and Fluorescent Properties of Deoxycytidine Analogues and Their Incorporation Into Oligonucleotides* **Elmehriki A. A. H.**, Suchy M., Wojciechowski F, Hudson R. H. E.

11:40 0124 *Stability of Imidazolidines and Stereospecific Synthesis of Quaternary Diamino Diacids* **Moozeh K.**, Kwon S.H., Chin J.

12:00 0021 *Synthesis of novel esters and quaternary amide salts of sym-triazine derivatives that could be potential acetylcholinesterase inhibitors and fibrillogenesis inhibitors of amyloid beta-peptides in Alzheimer's disease* **Liu AL**, Veloso AV, Mikhaylichenko SM

12:20 End of Session

Inorganic BSB-117

Chair: Peng Wang

09:40 0078 *The Synthesis and Reactivity of 4,5-diazafluorene and 4,5-diazafluorenide ligands* **Hughes S.**, Annibale V., Song D.

10:00 0005 *Towards Catalytic C-H Bond Stannylation with Cobalt and Platinum* **Matthews J.**, Johnson S.A.

10:20 0157 *Towards the Supramolecular Model for Vanadium Haloperoxidase* **Patel DP**, Bian L, Mikhaylichenko L, Zhang XA

10:40 Coffee Break

11:00 0138 *Generation of a carbene from 1,4-diaza-1,3-butadiene containing mixed sandwich cobaltocenes* **Asiedu E.**, Magdzinski E., Ragogna P.J.

11:20 0063 *Preparation and Reactions of a Novel Allyl Germylene π-Complex* **Leake J. D.**, Duffy I., Leigh W. J.

11:40 0105 *Design and Synthesis of Tetradentate β-diketiminate Ligands and their Boron Complexes* **Barbon S. M.**, Gilroy J. B.

12:00 0054 *Reactivity of -ketodiiminate ligands with molybdenum(V) oxidohalides* **Qi Y**, Hadzovic A

12:20 End of Session

Inorganic Materials BSB-121

Chair: Ian Duffy

09:40 0103 *Stabilizing non-existing RE_4Si_3 and RE_4Ge_3 binaries through the Valence Electron Concentration.* **Raiju Murugaanandan C.**, Yurij

10:00 0161 *Towards the Stable and Surface Active Metal Nanoparticles by the Surface Confined Cross-linking of Ligands* **Yu J. K.**, Eichhorn S. Holger

10:20 0159 *Utilization of bacterial cellulose aerogels as a scaffold for the synthesis of metal oxide catalysts* **Wisdom NW**, Vreugdenhil A, Strap J, Trevani L

10:40 Coffee Break

11:00 0011 *Novel Ferrocene-containing Dyes for Light Harvesting Applications* **Tulsiram N**, Koivisto B

11:20 0108 *Syntheses and physicochemical properties of ferrocene-BODIPY based dyes* **Pham T.**, Koivisto B.D.

11:40 0085 *Synthesis and photochromism of a silicon and germanium substituted dithienylethene ligand.* **Evans A**, Price J.T., Ragogna P.J.

12:00 0032 *Electron Spin Resonance Studies on the Dimerization of 1,2,3,5-Dithiadiazolyl Radicals* **Mohamud J.M**, Rawson J.M, Hayward J

12:20 End of Session

Cell Chemistry BSB-136

Chair: Leigh Spencer

09:40 0081 *Immunological detection of cytochrome b5 isoform I in Giardia lamblia* **Teghtmeyer M**, Rafferty S

10:00 0077 *Ubisol QE as a preventative treatment for MPTP induced neurodegeneration in DJ-1 deficient genetically susceptible mice model of Parkinson's disease* **Jasra H.**, Muthukumaran K., Smith J., Sikorska M., Sandhu J., Cohen J., Lopatin D., Pandey S.

10:20 0074 *Targeting Mitochondrial and Oxidative Vulnerabilities Using Synthetic Analogues of Pancratistatin in Breast Cancer* **Joshi S**, Ma D, Tarade D, Vshyvenko S, Hudlicky T, Pandey S

10:40 Coffee Break

11:00 0153 *Seeking the redox partners of Giardia lamblia cytochrome b_5* **Campanaro K.**, Rafferty S., Yee J.

11:20 0100 *Evaluating the Anti-Cancer Activity of Synthetic Analogues of Pancratistatin in Colorectal Cancer and Leukemia Cells and in Colon Tumor Xenografts* **Church J**, Ma D, Stokes K, Pandey S, Vshyvenko S, Hudlicky T

11:40 0130 *Characterization of cells with unusually high DNA content in the Giardia lamblia trophozoite cell cycle* **Horlock-Roberts K. A.**, Yee J.

12:00 0107 *Elucidating the Structure and Function of Streptomyces hawaiiensis ClpP proteases* **Patel P. K.**, Ortega J.

12:20 End of Session

Biomolecular BSB-138

Chair: Lana Kostina

09:40 0111 *SOYBEAN PEROXIDASE IMMOBILIZATION ON ORTHO-CRESOL POLYMERIC SOLIDS, AN AID TO ENZYME PRODUCTION* **Xiao Y.**, Feng W.

10:00 0087 *Design of a Tool for Photocontrol of Translation* Ariyakumaran R, Kumar A, **Jaikaran A.S.I.**, Woolley G.

10:20 0106 *Exploring The Silicon Substrate Tolerance of the Diatom Nitzschia curvilineata* **DeJong J.L.**, Zelisko* P.M.

10:40 Coffee Break

11:00 0016 *Isolation and Characterization of Catalytic DNA via Independent In Vitro Selection* **Gysbers RE**, Tram K, Li Y

11:20 0166 *Novel approach to detect Listeria monocytogenes* **Feng Q.**, Kanda P., Li Y.

11:40 0135 *Efficient Methods in Creating Hemoglobin Based Blood Substitutes* **Wang A**, Kluger R

12:00 0048 *Biochemical characterization of a novel MLH1 missense variant in the diagnosis of HNPCC* **Zhou A.**, Bell K., Zbuk K., Guarne A.

12:20 End of Session

Analytical BSB-137

Chair: Nadine Wellington

09:40 0162 *Microanalytical Separation in a Photonic Crystal Fiber* **Gibson N.**, Loock P.

10:00 0059 *The Effects of Low Molecular Weight Organic Acids on the Desorption of Lead from Natural Soils* **Cheyne C.A.**, Murphy J.G.

10:20 0018 *Competitive Binding of Ibuprofen and Perfluoroctanesulfonic Acid with Serum Albumin Studied by Electrospray Ionization Mass Spectrometry* **D'Alessandro ML**, Ellis DA, March RE

10:40 Coffee Break

11:00 0002 *Towards the development of a Sequencer-On-A-Chip for in-field Species Identification: On-Chip Isothermal Amplification of DNA Barcodes* **Udugama B.N.**, Gams M.S., Bialy R.N., Otieno W.A., Piunno P., Stefanovic S., Krull U.J., Barzda V.

11:20 0158 *Towards the development of a Sequencer-On-A-Chip for in-field Species Identification; Optimization of Sieving Matrix Formulations for On-Chip Sanger Sequencing.* **Bialy R.M.**, Gams M.S., Otieno W.A., Udugama B.N., Barzda V., Krull U.J., Piunno P.A.E., Stefanovic S.

11:40 0072 *Investigating the folding intermediates of Cytochrome c using Traveling Wave Ion Mobility Mass Spectrometry* **Hakimzadah S.**

12:00 0119 *Measuring the Dynamics of Schizosaccharomyces pombe La in the Absence and Presence of RNA, Using Time Resolved Mass Spectrometry and Microfluidics Enabled H/D Exchange.* **Shaikh A**, Wilson D.K.

12:20 End of Session

Physical BSB-115

Chair: Farnaz Heidarzadeh

09:40 0154 *Theoretical Modeling: For an Interfacial Fluorescence Resonance Energy Transfer in Quantum Dot Donor - Dye Acceptor Biorecognition System* **Wan K.**, Krull U.J.

10:00 0101 *Path integral simulations of hydrogen molecules trapped in water clathrate cages* **Cantin J. T.**, Zeng T., Schmidt M., Roy P.-N.

10:20 0080 *Accelerating quantum molecular dynamics simulations using graphical processing units* **Bishop K**, Faruk N, Schmidt M, Roy P.-N.

10:40 Coffee Break

11:00 0026 *Conformational Clustering of Peptide Met-enkephalin Employing a Self-Organizing Map With Toroidal Boundaries* **Gienow C.**, Gordon H.

11:20 0110 *Discrimination of Cysteine from Serine: A QM/MM Study on the Activation step of Cysteinyl-tRNA Synthetase.* **Kazim E.**, Fortowsky G. B., Gauld J. W.

11:40 0060 *Molecular modelling of folate-conjugated PSMA nanotubes for tumor-targeted drug delivery* **McTaggart M.R.**, Malardier-Jugroot C.

12:00 0029 *Coral Allene Oxide Synthase: A Mutagenic Computational Study* **De Luna P.**, Bushnell E.A.C., Gauld J.W.

12:20 End of Session

Mats./Spectroscopy BSB-120

Chair: Nicole DeAlmeida

09:40 0165 *Developing a fluorescently labelled bacterial microcrystalline cellulose substrate* **Palermo A**, Cranston E, Moran-Mirabal J

10:00 0099 *Spin Gymnastics: Using Specialized Radio-Frequency Pulses to Study Unreceptive Quadrupolar Nuclei* **Jaroszewicz M.J.**, Harris K.J., Johnston K.E., Schurko* R.W.

10:20 0047 *Combinatorial Colourimetric Sensing: Multidimensional Differentiation of Organic Liquids* **Chan A.S.**, Nerger B.A., Kinney M.H., Raymond K.P., Burgess I.B., Koay N., Aizenberg J.

10:40 Coffee Break

11:00 0044 *Dynamic Wetting and Colour in Photoresponsive Inverse Opal Films* **Nerger B.A.**, Burgess I.B., Singleton T.A., Goulet-Hanssens A., Koay N., Barrett C.J., Aizenberg J.

11:20 0040 *Oxide Nanoparticles for Functional Applications* **McEneny A.**, Cathcart N., Kitaev V.

11:40 0033 *Pressure-induced transformations of s-triazine and cyanuric triazide (CTA) probed by vibrational spectroscopy* **Till E**, Zhou L, Song Y

12:00 0012 *Developing Modern Undergraduate Laboratories: The Design of Light-Harvesting Dyes* Koivisto B, **Hussein B**, Fischer B, Pham T, Sammuelsson A

12:20 End of Session

Organic Materials BSB-119

Chair: Talena Rambarran

09:40 0102 *Benzimidazolium Based Molecular Shuttles* **Yu P**, Zhu K, Loeb S.J.

10:00 0112 *Synthesis and Characterization of New Liquid Crystalline Dibenzanthracenes* **Schneider A.**, Maly K.

10:20 0084 *Synthesis and Characterization Side-Chain Free Columnar Discotic Liquid Crystals* **Taing H.**, Eichhorn S.H.

10:40 Coffee Break

11:00 0091 *Synthesis of 6-oxotetrazane Polymers as Precursors for 6-Oxoverdazyl Radical Polymers* **Harrison C. S.**, Gilroy* J. B.

11:20 0137 *Synthesis of a Series of Novel Conjugated Polymers with Tunable Electronics via Strain-Promoted Azide-Alkyne Cycloaddition Reactions.* **Kardelis V**, Adronov A

11:40 0030 *Photodegradable Polymer Vesicles* **McIntosh J.T.**, Gillies E., Nazemi A.

12:00 0117 *Dissecting Colloidal Stabilization Factors in Crowded Polymer Solutions by Forming Self-Assembled Monolayers on Gold Nanoparticles* Lang N., **Liu B.**, Zhang X., Liu J.

12:20 End of Session

THE PHOENIX

12:20 Lunch

Saturday PM

BSB-147

2013 SOUSCC

Chair(s) - Chair

Organic BSB-147

Chair: Carlos Zepeda Velazquez

13:40 0164 *Diastereoselective Indium-Mediated Approach to Chiral $C_{(3)}$-Substituted Phthalides* **Curiel Tejeda J.E.**, Dudding T.

14:00 0020 *Regioselective functionalization of carbohydrates via borinic acid catalysis* Beale T., **Dobrovolsky D.**, Taylor M.

14:20 0014 *Solid-phase synthesis of peptidyl selenoesters for rapid native chemical ligation at difficult sites* **Ghassemian A.**, Alewood P.F., Durek T.

14:40 0093 *Regioselective Functionalization of 7-azaindole and Isomeric Derivatives* **Kaye M.**, Dalziel M., Kitching M., Schneider C., Snieckus V.

15:00 Coffee Break

15:20 0070 *Towards the Total Synthesis of (±)-Paralycolin A* **Lee C.-H. F.**, Guimarães K. G., Hurst T. E., Kitching M. O., da Silva A. J. M., Snieckus V.

15:40 0043 *Towards the Total Synthesis of Isoprekinamycin and the Related Fluostatin Natural Products* **Ziebenhaus C. A.**, Kitching M. O., Jignesh P., Snieckus V.

16:00 0160 *Synthesis of aza-analogues of narciclasine* **Rodriguez P.**, Vshyvenko S., Hudlicky T.

16:20 0145 *Towards the Total Synthesis of Lysergic Acid via Rh-Catalyzed Asymmetric Ring Opening* Tsoung J., **Lui E. K. J.**, Boyer A., El-Salfiti M., Lautens M.

16:40 End of Session

Inorganic BSB-117

Chair: Lucia Myongwon Lee

13:40 0140 *Carbonyl Sulfide Decomposition on Cationic Rhodium Clusters* **Chow W.C.T.**, Lecours M.J., Hopkins W.S.

14:00 0152 *Towards the Syntheses of Mercury(IV) Compounds* **DeBackere J.R.**, Mercier H.P.A., Schrobilgen G.J.

14:20 0009 *Migration Insertion Polymerization: A New Concept for Main Chain Metal Containing Polymers.* **Tsang B.**, Cao K., Liu Y., Wang X.

14:40 0150 *Ru(II)-EDTA complex as a water, acid and high-temperature stable deoxygenation catalyst* **Sullivan R**, Schlaf M

15:00 Coffee Break

15:20 0097 *Synthesis and investigation of novel thermoelectric suboxides:* $Gd_2Bi_{1-x}Sb_xO_2$, $Sm_2Bi_{1-x}Sb_xO_2$, $Ho_2Bi_{1-x}Te_xO_2$ **Ogilvie L. J.**, Mozharivskyj Y.

15:40 0121 *Targeting Fluorinated Organic Molecules via Perfluorometallacycle Activation* **Andrella N.O.**, Baker R.T.

16:00 0046 *A Mechanistic Investigation of H/D Exchange of Unactivated C-H bonds from a Pentanuclear Nickel Cluster* **Shoshani M**, Johnson S.A

16:20 0142 *Catalytic and Mechanistic Studies of Hydrosilylation Mediated by a Zinc Hydride Complex* **Boone C.**, Nikonov G.I.

16:40 End of Session

Inorganic Materials BSB-121

Chair: Chris Gendy

13:40 0118 *Comparative study of three ruthenium (II) polypyridyl complexes in dye-sensitized solar cells* **Abner S.**, Morin S., Sepehrifard A.

14:00 0051 *Microsolvation of Uranyl, UO2+* **Hasan M**, Baldwin J, Hopkins S.W.

14:20 0094 *Investigating the Adsorption of Organic Compounds in MOF MIL-53* **Ibrahim B.**, Xu J., Huang Y.

14:40 0023 *Insertion Complexes of Cyclic Organic Molecules Trapped in Metal-Halide Ion-pairs* **Cochrane B.S.**, Naumkin F.Y.

15:00 Coffee Break

15:20 0028 *Synthesis of dipyrazinyl ketone by transmetalation of 2-tributylstannanyl pyrazine* **Emberson K.**, Metallinos* C., Stamatatos T.

15:40 0004 *Characterization of Metal-Organic Framework using Solid-State ^2H NMR and X-ray Absorption Spectroscopy* **Sinelnikov R.**, Xu J., Sham T.K., Huang Y.

16:00 0104 *Binding Manganese to Metallothionein* **Assaf M.**, Stillman M.

16:20 0098 *Alkali-Metal Derivatives of Highly-Charged Conjugated Anions* **Somasundaram V.**, Vargas-Baca I.

16:40 End of Session

Cell Chemistry BSB-136

Chair: Lukas Sadowski

13:40 0141 *A Novel Function of Cystathionine-ϒ-lyase: Disulfide Reductase* **Atwan Y.**, Faccenda A., Mutus B.

14:00 0019 *Investigation of the effect of glutamine and its metabolites on the phosphorylation of mTORC1 targets* **Desmarais G**, Abusneina A, Gauthier E

14:20 0131 *Functional consequences of NOx-modification on cystathionine-γ-lyase.* **Ali Khan H**, Faccenda A, Wang J, Mutus B

14:40 0096 *DAHP Synthase: Oxime Inhibition and Dynamic Studies on an Antibiotic Target* **Curiel Tejeda E.J.**, Berti P.J.

15:00 Coffee Break

15:20 0134 *Identifying novel natural product inhibitors of the 1-deoxy-D-xylulose 5-phosphate pathway.* Chung T.E., Czarny T., **Brown E.D.**

15:40 0037 *The Impact of Cis-Regulatory Variation on Drosophila melanogaster Malic Enzyme Biochemistry* **Gallagher K**, Merritt T

16:00 0066 *Expression and purification of Bacterial Cellulose Synthase Protein E from Escherichia coli* **Kell L.F.**, Jelokhani-Niaraki M., Weadge J.T.

16:20 0067 *Hisactophilin: The Adventures of the Truncation Mutant, L76A* **Tran E**, MacKenzie D, Meiering E

16:40 End of Session

Biomolecular BSB-138

Chair: Madiha Khan

13:40 0151 *Investigating the dimerization interface in the RR protein VraR through a single point mutation.* Golemi-Kotra D., **Gagarina V.**

14:00 0128 *HDAC4 interaction with Myocyte Enhancer Factor 2 (MEF2)* **Aram R,**

Wales S, McDermot JC

14:20 0034 *Structural and Functional Analysis of the Bcs C protein from the Bacterial Cellulose Protein Complex in Escherichia coli* **Skrinjaric J.P.**, Slawson R, Horsman G, Weadge J.T.

14:40 0149 *Docking Study on Giardia Flavohemoglobin* **Eisner M.**, Gordon H., Rafferty S., Yee J.

15:00 Coffee Break

15:20 0075 *Metabolic Optimization of Potent Small Molecule Inhibitors of Stat3 Dimerization* **Mac S.**, Arpin C.C., Gunning P.T.

15:40 0109 *The Effect of pH and Chemical Denaturants on the Structure and Metal Status of Anthrax Lethal Factor* **Mapletoft J.**, Siemann S.

16:00 0092 *An investigation into the molecular mechanism of human uncoupling protein-2 anion and proton transport* **Parker JP**, Hoang T, Matovic T, Smith MD, Jelokhani-Niaraki M

16:20 0071 *Analysis of DAHP Oxime as a Transition State Mimic of DAHP Synthase* **To F.**, Balachandran N., Berti P. J.

16:40 End of Session

Analytical BSB-137

Chair: Yujie Zhu

13:40 0113 *Effects of Ammonium Bicarbonate on the Electrospray Ionization Mass Spectra of Proteins* **Hedges J.**, Vahidi S., Konermann L.

14:00 0095 *Correlation of photobleaching, oxidation and metal induced fluorescence quenching of DNA-templated silver nanoclusters* **Morishita K.**, MacLean J., Liu B., Jiang H., Liu J.

14:20 0027 *Expanded Newborn Screening with Chemical Derivatization by MS/MS* **Saoi M.**, Britz-McKibbin P.

14:40 0055 *Paper Based Solid-Phase QD-FRET Nucleic Acid Hybridization Assay* **Shahmuradyan A**, Noor O. M., Krull U. J.

15:00 Coffee Break

15:20 0068 *Rapid time-scale dynamics and structure of Abeta(1-40) interacting with micelles* **Tawadrous S.**

15:40 0126 *Methods for small-volume analysis of phosphopeptides using magnetic beads* **Thompson A. A.**, Yeung K. K. C.

16:00 0056 *Development towards a semi-quantitative paper-based immunoassay for eosinophil peroxidase.* • **Yin K**, Sicard C, Brennan JD

16:20 0013 *Synthesis and testing of an activity-based elemental tag for O-GlcNAcase* **Lumba M.A.**, Cao P., Nitz M.

16:40 End of Session

Physical BSB-115

Chair: Dinesh Basker

13:40 0053 *An Evaluation of Regions of Flexibility in the F-Spondin Reeler Domain Using Molecular Dynamics Simulations* **Stromski K**, Madarati A, Gordon H

14:00 0010 *Reduction of Hydrogen Peroxide via Archaeal Thioredoxin Peroxidase: A Mechanistic DFT Investigation* **Simard D.J.**, Dokainish H., Gauld J.W.

14:20 0133 *Polarizability Calculations of Linearly Conjugated Systems Using Matrix Product States* **Kim T.**, Limacher P., Ayers P., Wouters S., Neck D.V.

14:40 0057 *Electronic Properties of Probed Polyaromatic Heterocycles by DFT Calculations* **Beiraghi O.**, Eichhorn S.H., Gauld J.W.

15:00 Coffee Break

15:20 0017 *Liquid Metal for use as Dynamic Electrode in Intrinsically Stretchable Devices* **Prochazka P. J.**, Amyotte S, Carmichael T. B.

15:40 0052 *The Electrochemical Monitoring of the Degradation Process of Fuel Cell Catalysts using Electrochemical Impedance Spectroscopy* **Reid O.**, Saleh F.S., Easton E.B

16:00 0147 *Understanding and Preparation of Sharp Metallic Tips Via Electrochemical Etching* **Awez Mohammad A.**, Wang Y., Kruse P.

16:20 0015 *Electrochemical and Microscopic Investigation of the Corrosion Behaviour of Mg AM50 Alloy* **Binns W. J.**, Asmussen R. M., Jakupi P.

16:40 End of Session

Mats./Spectroscopy BSB-120

Chair: Nicole Rice

13:40 0065 *Controlling the Adsorption of DNA to Nanoceria* **Pautler R.**, Huang P. J-. J., Cao J., Liu B., Liu J.

14:00 0122 *Synthesis and Characterization of Amphiphilic Nanoparticles* **Zghal O.**, Eichhorn S.H.

14:20 0089 *Shape Control in Noble Metal Nanoparticles: Silver Icosahedra and Gold Stars* **Keunen R**, Cathcart N, Macoretta D, Kitaev V

14:40 0086 *Synthesis of shell isolated nanoparticles for plasmon enhanced spectroscopy* **Chen W**, Aroca R

15:00 Coffee Break

15:20 0069 *Light-Activated Metal-Coordinated Supramolecular Complexes with Charge-Directed Self-Assembly* **Lopez A**, Liu J

15:40 0038 *Photoelectrochemical Enhancement of $CuInS_2$ Light-Absorbing Layers for Solar Cells.* **Hart C.**, Tapley A., Ding Z.

16:00 0088 *Determining the Limit of Detection of a Platform Fabricated by Nanosphere Lithography Used for Surface-Enhanced Raman Spectroscopy* **Wallace G**, Tabatabaei M, Lagugné-Labarthet* F

16:20 0129 *^{35}Cl SSNMR of HCl Pharmaceuticals: Pills, Polymorphs and Pure Forms* **Namespetra A.M.**, Sandre A.R., Harris K.J., Hildebrand M.P, Schurko R.W.

16:40 End of Session

Organic Materials BSB-119

Chair: Laura Dodge

13:40 0024 *Molecular Imaging of Cancer Using Dendritic Scaffolds* **Colaneri C.**, Sadowski L., Adronov A.

14:00 0148 *Selective Coating of T4 Bacteriophage through Controlled Silica Growth* **Kurian J**, Brook MA, Khan MF

14:20 0031 *Enzyme-mediated synthesis of siloxane-containing chiral polymers* **Séguin J.P.**, Zelisko P.M.

14:40 0125 *Thin Polymer Films as Cell Matrices* **Sriskandha S.E.**, Burke N.A.D., Stover H.D.H.

15:00 Coffee Break

15:20 0146 *A Controlled Synthesis of Polyoxothiazene-Polyphosphazene block-co-polymers* **Al-Faouri T**, McWilliams A.R, Foucher D.A

15:40 0156 *Electrospun Conductive Nanofibres from Poly(ethylene oxide) Doped with Single-Walled Carbon Nanotube-Conjugated Polymer Constructs* **Naeem F.**, Adronov A., Moran-Mirabal J.

16:00 0083 *Stability of Aqueous Nanodroplets Containing RNA Complex* Malevanets A., Constas S., **Turnbull M.**

16:20 0127 *Solvent Recyclability in the Undergraduate Organic Laboratory* Dicks A.P, **Stacey J.M**

16:40 End of Session

From **17:30** until **18:30**

outside CIBC HALL

17:30 Poster Session

0090 *Microwave Assisted Functionalization of Water-Soluble, Size Separated Silicon Quantum Dots* **Chen K.**, Mastronardi M., Ozin G. A.

0064 *An Extended Study of the Effect of Betadine on Silicone Elastomers* **Urlich T.R.**, Brook M.A.

0115 *Towards Allyation/Oxidation Protocols for C3 Functionalized Indoles with Potassium Organotrifluoroborates* **Menzies P.**, Batey R.A.

0045 *A Simple Synthesis of β-Aminocarbonyl Compounds from Alkenes and Hydrazones* Moon P. J., Gan W., Clavette C., Das Neves N., Markiewicz T., Toderian A., **Beauchemin A. M.**

0025 *The Synthesis of Modified Organic Dyes for Direct Integration into a Hole-Transport Material.* Koivisto B, **Abdi O**, Bonnier C, Machin D

0114 *Studies Toward a Wittig Olefination Route to γ-Functionalized Z-allyltrifluoroborates* **Dalesandro D.A.**, Beveridge R.E., Batey R.A.

0042 *Synthesis and Self-assembly of PFS-b-PMMA Diblock Copolymers* **Lin K.X.**, Zhang M., Winnik M.A.

0050 *Controlling the wettability of acrylate polymers* **Chen Y.**, Khan M.F., Delhorbe V., Brook M.A.

0139 *The Synthesis of Heptiptycene Derivatives for Use in Host-Guest Chemistry* **Ellis D.A.M.**, Maly K.E.

0120 *Synthesis of Ferrocene-Cysteine Derivatives* **Lin Y.-C.**, Kraatz H.-B.

0123 *Deposition of Silver nanoparticles on cellulosic substrates for biomedical applications* **Scott C.**, Strap J., Trevani L

0073 *Controlled Encapsulation of Gold Nanoparticles by Escherichia coli Bacterioferritin* **Taylor R. M.**, van der Ven A., Honek J.

0155 *Isolation and Purification of Voltage-Dependent Anion Channel (VDAC) in Mouse Myelin* **Bhatia MB**, DeBruin L

0144 *Interrogating p19-small RNA Interactions with Small Molecules* **Filip R.**, Danielson D.C., Pezacki J.P.

0143 *Soraphen A-Mediated Inhibition of Acetyl CoA Carboxylase Activity Represses Hepatitis C Replication* **Desrochers G**, Singaravelu R, O'Hara S, Srinivasan P, Pezacki J

0136 *Transfer of Chemical Moieties to Biomolecules Using S-Adenosyl-L-Methionine Dependent Methyl Transferases* **Kay TM**, Myers CL, Honek JF

0132 *Investigating Phosphonate in the Metagenome* **Taglione M**, Horsman G

0116 *Synthesis of Probes for the Activity-Based Profiling of Lipid Kinases* **Cornacchia C. A.**, Hunt A. D., Sherratt A., O'Hara S., McKay C. S., Pezacki J. P.

0079 *H477R PEPCK Alternates Ω loop Lid Domain Interaction Characterized Through Kinetic Studies* **Cui D**, Holyoak T

0082 *Structural and functional characterization of ClpP1-4 in acyldepsipeptide producing Streptomyces hawaiiensis* **Desai H**, Xing L, Patel P, Homchaudhuri L, Alexopoulos J, Ortega J

0061 *A Biosensor: The Ability of a Histidine Peptide to Coordinate Metal Ions* **Cao Y**, Kraatz H.-B.

0062 *Evaluating the refolding interactions of hisactophilin, a myristoylated protein* **Lemke M.**, MacKenzie D., Smith M., Meiering E.

0049 *Heterologous Production and Characterization of hSRCR1* **Huynh A.**, Dorrington M., Rivet L., Yin C., Bowdish D., Guarne A.

0036 *Novel protein-based siRNA-delivery agents and their enhancement through promoting endosomal escape.* **Wang W.**, Danielson D.C., Sachrajda N., Pezacki J.P.

0008 *Optimising Giardia lamblia cytochrome b_5-I expression conditions in minimal media as a prelude to structural 2-D NMR spectroscopy* **Mesbahuddin M.S.**, Rafferty S., Yee J.

0022 *Synthesis of Truncated Stat3 Inhibitors for Anticancer Therapy* **Colaguori R.**, Page B. D. G., Gunning P.T.

0006 *Investigating the use of bacteriophage M13 pVIII protein in biomaterials applications* **Rowan C.**, Petrie A., Daub E., Honek J.F.

End of Session

CIBC HALL

18:30 BANQUET

The presentation of awards will take place after 9:00 pm.

21:30 End of banquet and conference.

ABSTRACTS

1 09:40 Saturday BSB-147

Synthesis of novel 1,2-dihydropyridazine-3,6-dione derivatives of 1,3,5-sym-traizine and screening for their antimicrobial activity **M Thakkar** <*mauli.thakkar@mail.utoronto.ca*> and **L Mikhaylichenko** <*mikhay@utsc.utoronto.ca*>, University of Toronto Scarborough.

The capacity to form diverse array of biologically active compounds has made 1,3,5-triazine a commonly used reagent for organic synthesis. In search of the compounds that encompass this property of sym-triazine, various di-substituted derivatives were synthesized from cyanuric chloride, with substituents on C4 and C6 positions. Methoxy, piperidinyl, and pyrrolidinyl groups were used as substituents at C4 and C6 positions which are known to possess antimicrobial activities. These mono-chloride sym-triazine derivatives were subsequently converted into hydrazine derivatives through quaternary triethylammonium salt. The synthesized hydrazine derivatives were allowed to undergo cyclization reaction where citraconic anhydride completed the ring formation through cyclo-addition mechanism. The overall yields of synthesized 1,2-digydropyridazine-3,6-diones were between 50 and 65%. The structures of the synthesized compounds were confirmed using IR, 1H-NMR, and Mass spectrum analysis. Analysis of potential bioactivities of these and previously synthesized novel derivatives of symtriazine is under progress.

2 10:00 Saturday BSB-147

Designing and Synthesizing Bimodal, Di-Salicylic Acid PTP Inhibitors **P.T Gunning** <*patrick.gunning@utoronto.ca*>, **S.H Haftchenary** <*s.haftchenary@utoronto.ca*>, **D.B Ball** <*dan.ball@utoronto.ca*> and **A.J Jouk** <*andriana.jouk@mail.utoronto.ca*>, University of Toronto, Mississauga, Ontario, L5L 1C6.

Bimodal PTP inhibitors have been identified as potentially significant therapeutic drugs by structure-based design, utilizing differences in accessibility to peripheral sites among these imperative regulators of dephosphorylation. We have determined that our bimodal di-salicylic acid inhibitors target PTP1B, Tc-PTP and PTPσ with single digit μM potency but expectedly no selectivity. Herein, we report the start of the design and synthesis of our second-generation bimodal PTP inhibitors that feature an extended salicylic acid on the core scaffold. These molecular inhibitors have been designed to incorporate various linkers that extend the second salicylic acid present on our current most potent inhibitors to date. Our hope is that this new line of compounds will be both more potent and observe greater specificity within the large family of PTPs. Ultimately, this study has enabled us to report our progress in the development and synthesis in the search of more potent, selective and unique PTP inhibitors with applications towards therapeutically treating disease associated with the activity of PTP.

3 10:20 Saturday BSB-147

Structure determination and application of peptide macrocycles from aziridine aldehydes **S Ler** <*spencer.ler6@gmail.com*>, **S Zaretsky** <*serge.zaretsky@utoronto.ca*>, **C White** <*cwhite@chem.utoronto.ca*>, **C Scully** <*cscully@chem.utoronto.ca*> and **A Yudin** <*ayudin@chem.utoronto.ca*>, University of Toronto, 80 St. George St., Toronto, ON., M5S 3H6.

Cyclic peptides have garnered enormous interest as scaffolds that rigidify amino acid sequences into predictable conformations. These macrocycles have seen applications as imaging agents, nanomaterials, and therapeutics. However, synthesis of cyclic peptides from their linear precursors is afflicted by both kinetic and thermodynamic challenges, resulting in low yields and stereoselectivity. Through the use of amphoteric aziridine aldehydes, we recently reported a facile method to synthesize cyclic peptides via an intercepted Ugi reaction. The reaction is performed with unusually high concentrations (0.1 M), creating heterodetic cyclic peptides with high stereoselectivity and no creation of oligomeric products. Investigations towards the stereochemistry within the artificial linker introduced were performed. Further structural information of these peptide macrocycles was obtained by a crystal structure, which allowed for a rational design of peptide scaffolds towards the inhibition of calpain, a signaling protease whose excitotoxicity is implicated with neuronal death. To further optimize interactions with our lead inhibitor and calpain, a library of 21 cyclic peptides was synthesized using our technology.

4 11:00 Saturday BSB-147

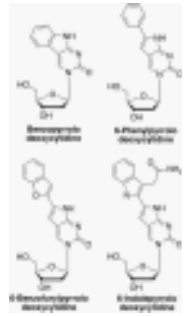
Parallel synthesis of a diverse library of pyridinone based compounds to probe the chemical space of binding to L-glutamine: D-fructose-6-phosphate Amidotransferase (GFAT) **B.S. Bagha** <*baghabs@mcmaster.ca*>, **L.A. Walter** <*waltel@mcmaster.ca*> and **A. Capretta** <*capretta@mcmaster.ca*>, McMaster University.

The hexosamine biosynthetic pathway (HBP) plays an important role in the development of insulin resistance and further diabetic complications. The enzyme L-glutamine: D-fructose-6-phosphate Amidotransferase (GFAT) is the first and rate-limiting step of the HBP and has been identified as a novel target for inhibition. Amrinone, a pharmaceutical used to treat congestive heart failure, was identified as GFAT inhibitor with an IC50 of 8.9-84uM. In order to develop a more potent and selective inhibitor, the skeleton and appendages of the pyridinone core should be altered for the greatest chemical diversity. A parallel synthetic method has been designed around the Suzuki coupling of different iodinated pyridinone scaffolds and a variety of aromatic boronic acids. This optimized method allows for the potentially automated synthesis of a large library of diverse compounds. The expected synthesis of over 30 compounds will give a preliminary understanding of the chemical space of the binding site, and how to further develop a more potent and selective inhibitor of GFAT.

5 11:20 Saturday BSB-147

Synthesis and Fluorescent Properties of Deoxycytidine Analogues and Their Incorporation Into Oligonucleotides **A. A. H. Elmehriki** <*aelmehri@uwo.ca*>, **M. Suchy**, **F Wojciechowski** and **R. H. E. Hudson** <*rhhudson@uwo.ca*>, Department of Chemistry, The University of Western Ontario, London, Ontario Canada N6A 5B7.

Fluorescence spectroscopy presents a powerful environmentally sensitive technique that through the design of fluorescent probes can elucidate the function of nucleic acids.[1] In terms of the use of nucleobase analogues as fluorescent probes several intrinsically fluorescent analogues capable of participating in hybridisation have been developed[2], although useful improvements in sensitivity or specificity are still required. Herein we describe the synthesis and fluorescent properties of 6-phenylpyrrolodeoxycytidine[3], 6-indolepyrrolodeoxycytidine, 6-benzofurylpyrrolodeoxycytidine and benzopyrrolodeoxycytidine[4] leading to the incorporation of 6-benzofurylpyrrolodeoxycytidine and benzopyrrolodeoxycytidine into oligonucleotides.

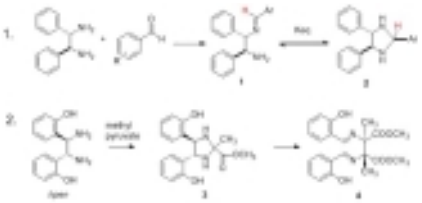


1. Kaul, M.; Barbieri, C. M.; Pilch, D. S. *J. Am. Chem. Soc.* **2004,** 126, 3447.
2. Dodd, D. W.; Hudson, R. H. E. *Mini-Rev. Org. Chem.* **2009,** 6, 378.
3. Hudson, R. H. E.; Ghorbani-Choghamarani, A. *Synlett* **2007,** 6, 0870.
4. Matteucci, M. D.; von Krosigk, U. *Tetrahedron Lett.* **1996,** 37, 5057.

6 11:40 Saturday BSB-147

Stability of Imidazolidines and Stereospecific Synthesis of Quaternary Diamino Diacids **K. Moozeh** <*kimia.moozeh@mail.utoronto.ca*> and **J. Chin** <*jchin@chem.utoronto.ca*>, Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6, Canada,; **S.H. Kwon**, , Department of Chemistry, College of Natural Sciences, Seoul National University, Seoul 151-747, South Korea .

1.Imidazolidines (2, 3) are intermediates in the synthesis of chiral diamines by diaza-Cope rearrangement (4). Thus it is important to understand factors affecting the stability of imidazolidine rings. This study explores the steric and electronic effects on the stability of the imidazolidine rings using both the Hammett equation and DFT computations. There is an excellent correlation between the values of the equilibrium constants for the imidazolidine ring formation obtained by ^{1}H NMR methods and computational energy differences between the imidazolidines and their ring-opened monoimines.



2.A wide variety of chiral vicinal diamines can be synthesized stereospecifically using *hpen* and aryl/alkyl aldehydes. However up to date it has been a challenge to synthesize chiral vicinal diamines exclusively from ketones and *hpen*. Here the first such example using methyl pyruvate as the ketone for stereospecific synthesis of a diamino diacid with two quaternary chiral centers is reported.

7 12:00 Saturday BSB-147

Synthesis of novel esters and quaternary amide salts of sym-triazine derivatives that could be potential acetylcholinesterase inhibitors and fibrillogenesis inhibitors of amyloid beta-peptides in Alzheimer's disease
AL Liu <*09liuamy@utsc.utoronto.ca*>, **AV Veloso** <*veloso@mail.utoronto.ca*> and **SM Mikhaylichenko** <*mikhay@utsc.utoronto.ca*>, University of Toronto Scarborough.

Novel sym-triazine compounds are formulated in this study that could be potential acetylcholinesterase inhibitors and fibrillogenesis inhibitors of amyloid beta-peptides (A) in Alzheimer's disease. Alzheimer's disease (AD) is the most common type of dementia and can affect memory, perception, emotional behaviour and cognitive abilities and worsens as time progresses. Currently there is no cure and no known cause for AD. The two main characteristic hallmarks of an AD brain are neuronal senile plaques and neurofibrillary tangles. Recent AD drug therapy is engaged in finding compounds which can affect multiple targets and thus have the potential to treat several diseases, known as multiple-target directed ligands (MTDL) (Cavalli). Previous studies conducted by Veloso et al. (2011) have confirmed that tri-substituted sym-triazine derivatives (TAE-1 and TAE-) can act act as A-aggregation modulators, -sheet fibril formation inhibitor and acetylcholinesterase (AchE) inhibitors through square-wave voltammetry (SWV) and ThT fluorescence spectroscopy. The esters synthesized in this study are based off TAE1 and TAE2. The new esters (Amide 1 and Amide 2) were synthesized with 24% and 55% yield respectively. A novel compound being made this year consists of a similar sym-triazine core but with fluorine atoms attached so the progress of the molecule can be monitored by Fluorine-19 NMR in the brain. Compounds inhibitory activity will be tested through ThT fluorescence spectroscopy and electrochemical studies.

8 09:40 Saturday BSB-117

The Synthesis and Reactivity of 4,5-diazafluorene and 4,5-diazafluorenide ligands
S. Hughes <*sarahj.hughes@utoronto.ca*>, **V. Annibale** <*vannibale@chem.utoronto.ca*> and **D. Song** <*dsong@chem.utoronto.ca*>, Davenport Chemical Laboratories, 80 St. George St., University of Toronto, Toronto, Ontario, M5S 3H6.

Diazafluorene (LH), and the corresponding anionic diazafluorenide (LH^-) ligands are predominantly bidentate N-donor ligands, but have also shown coordination with the C-donors from the central cyclopentadienyl-like ring. Based on structural similarities to the well-known "Nacnac" anionic ligand, which has previously been shown to afford the formation of a variety of metal coordination complexes[1], the reactivity and coordination chemistry of the substituted diazafluorenide ligand were investigated. Initial findings that have already been reported, include use of the LH^- ligand in hydrogenation catalysis[2,3], and from the compound $[RuCl_2(LH)(PPh_3)_2]$, findings include the air-oxidation of the CH_2 group of the central cyclopentadienyl-like ring[4], as well as long-range reversible splitting of H_2[5]. Assuming this reactivity is due in fact to the unquenched basicity on the anionic ligand combined with the Lewis acidity of the metal center, it seems plausible that there is further potential for small molecule reactivity, as will be discussed.

[1]Bourget-Merle, L.; Lappert, M. F.; Severn, J. R., *Chemical Reviews,* 2002, **102**, 30313066.
[2]Jiang, H.; Song, D. *Organometallics*, 2008, **27**, 3587-3592.
[3]Jiang,H.; Stepowska, E.; Song, D. *European Journal of Inorganic Chemistry*, 2009, 2083-2089.
[4]Jiang, H.; Stepowska, E.; Song, D. *Dalton Transactions*, 2008, 5879-5881.
[5]Stepowska, E.; Jiang, H.; Song, D., *Chemical Communications*, 2010, **46**, 556-558.

9 10:00 Saturday BSB-117

Towards Catalytic C-H Bond Stannylation with Cobalt and Platinum
J. Matthews <*matthewj@uwindsor.ca*> and **S.A. Johnson** <*sjohnson@uwindsor.ca*>, Department of Chemistry and Biochemistry, University of Windsor, Windsor, ON, N9B 3P4.

Nickel complexes have previously been shown to be effective in C-H bond activation and stannylation of fluorinated arenes.[1] The stannylation products are of synthetic use as reagents in Stille coupling reactions. Here, the use of cobalt and platinum is investigated in an effort to broaden the scope of substrates accessible by this process. Early results show that both Co and Pt facilitate C-H activation and stannylation, however only in very low turnovers. By gaining more mechanistic insight into how Co facilitates this reaction, the design of more effective complexes and the determination optimal reaction conditions can be targeted.

1. Doster, M. E.; Hatnean, J. A.; Jeftic, T.; Modi, S.; Johnson, S. A., *J. Am. Chem. Soc.* **2010,***132* (34), 11923-11925.

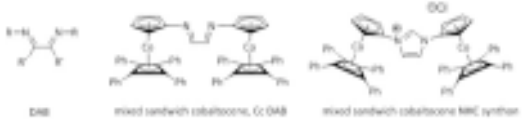
10 10:20 Saturday BSB-117

Towards the Supramolecular Model for Vanadium Haloperoxidase
DP Patel <*deepalk.patel@mail.utoronto.ca*>, **L Bian** <*libo.bian@mail.utoronto.ca*>, **L Mikhaylichenko** <*mikhay@utsc.utoronto.ca*> and **XA Zhang** <*xazhang@utsc.utoronto.ca*>, University of Toronto Scarborough.

Vanadium haloperoxidases (VHPOs) catalyze the oxidation of halides using orthovanadate anion (HVO_4^{2-}) as a cofactor, producing various halogenated natural organic products, many of which are of pharmacological interest. VHPO protein binds orthovanadate through hydrogen bonding, coulombic interactions and a single V-N coordination bond. We are interested in modeling the unique supramolecular structural features as well as the catalytic activity of VHPOs. Four structural models of VHPOs were prepared, all based on a tripodal ligand structure which mimics the non-covalent anion binding pocket at the active site of the enzyme. The fundamental structure of the vanadate receptor contains a central nitrogen bound to three positively charged guanidium groups substituted with hydrophobic alkyl and aryl groups (propyl, pentyl, dodecyl and benzyl). Considering previous work demonstrating that a pyrene-substituted analogue bound the vanadate dimer, the objective is to determine the substituents that will allow the selectively binding of the vanadate monomer, which is the enzyme cofactor. The derivatives were prepared with *tris*-(2-isothiocyanate-ethyl)amine which was converted into a substituted thiourea intermediate (yield: 70 90 %). The thiourea intermediate was selectively methylated at the sulfur with the protection of the central nitrogen by protonation, producing S-methyl isothiourea derivatives (yield: 72 80 %). The substitution reactions of S-methyl isothiourea with amine produces the final guanidium salt derivatives. Furthermore, the attempt to titrate the structural mimics with orthovanadate is under progress, to assess their fidelity as structural and functional models of VHPOs.

11 11:00 Saturday BSB-117

Generation of a carbene from 1,4-diaza-1,3-butadiene containing mixed sandwich cobaltocenes
E. Asiedu <*easiedu@uwo.ca*>, **E. Magdzinski** <*emagdzin@uwo.ca*> and **P.J. Ragogna** <*pragogna@uwo.ca*>, Department of Chemistry, Western University, 1151 Richmond Street, London, Ontario N6A 5B7.

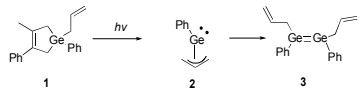


In the exploration of redox active ligands, the incorporation of inorganic groups into conventional organic-based frameworks is not uncommon. The 1,4-diaza-1,3-butadiene (DAB) ligand is one such ligand which exists as a part of a variety of compounds[1-2]. Often created from a DAB precursor, N-heterocyclic carbenes (NHCs) containing redox active functionalities have been used as ligands capable of imposing electrochemical switchable reactivity. Although there has been success in using ferrocene[3] in this regard, other metallocenes have been far less studied. Recently the Ragogna group has synthesized a DAB with pendant mixed sandwich cobaltocenes and reviewed its redox properties. As an extension of this work, we have synthesized a novel imidazolium salta precursor to an NHC. The synthesis and characterization of this chemistry will be detailed.

1.Trifonov, A. A.; Fedorova, E.A.; Ikorskii, V.N.; Dechert, S.; Schumann, H.; Bochkarev, M.N.; Eur. J. Inorg. Chem. 2005, 2812-2818
2.Bildstein, B.; Malaun, M.; Kopacka, H.; Fontani, M.; Zanello, P. Inorg. Chim. Acta 1999, 300, 16-22.
3.Butler, D.C.; Richards, C.J. Organometallics. 2002, 21, 5433-5436.

12 11:20 Saturday BSB-117

Preparation and Reactions of a Novel Allyl Germylene π-Complex
J. D. Leake <*leakejd@mcmaster.ca*>, **I. Duffy** <*duffyi@mcmaster.ca*> and **W. J. Leigh** <*leigh@mcmaster.ca*>, Department of Chemistry and Chemical Biology, McMaster University, 1280 Main Street West, Hamilton, ON Canada L8S 4M1.



A recent study by Leigh et al.[1] has provided insight into the unique interaction between germylenes and alkenes, and presents evidence for a novel π-complex between these two functionalities. To further study this interaction, a germanium compound, 1-allyl-3-methyl-1,4-diphenyl-1-germacyclopent-3-ene (**1**) has been synthesized, and contains an intramolecular alkene group. The photochemical excitation of **1** exhibits a short lived transient at λ_{max}=310 nm, assigned to the allyl germylene π-complex (**2**). Subsequently, the germylene decays to form digermene (**3**). Product studies of **1** in the presence of alcohols yields propene and an alkoxy-substitued product formed through a hydrogen transfer mechanism. Conversely, in the presence of acetic acid, **2** undergoes an insertion reaction while retaining its allyl side chain. These assignments and conclusions are supported by computational modeling.

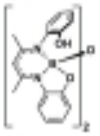
(1) Billone, P. S.; Beleznay, K.; Harrington, C. R.; Huck, L. A.; Leigh, W. J. J. Am. Chem. Soc. 2011, 133, 10523-10534.

13 11:40 Saturday BSB-117

Design and Synthesis of Tetradentate β-diketiminate Ligands and their Boron Complexes **S. M. Barbon** <*sbarbon@uwo.ca*> and **J. B. Gilroy** <*joe.gilroy@uwo.ca*>, Department of Chemistry and Centre for Advanced Materials and Biomaterials Research, University of Western Ontario, London, ON, Canada, N6A 5B7.

β-diketiminates are a well known class of ancillary ligands commonly encountered in the field of coordination chemistry.[1] They typically have two aryl substituents, which can be modified to increase their steric bulk, making them ideal for stabilizing low valent metal centres.
Very few known β-diketiminate complexes contain heteroatoms on the aryl substituents (e. g. **1**). We believe by including heteroatoms, we can form ligands with potentially tetradentate binding pockets which will benefit from the increased stability associated with the chelate effect. Direct synthesis of the target ligand **1** proved difficult, so protection strategies were employed. The use of BBr_3 as a demethylation agent yielded a novel Boron complex **2**. The synthesis and characterization of this and related boron complexes will be discussed in this presentation.

1



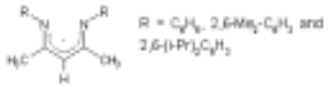
2

1. Bourget-Merle, L.; Lappert, M. F.; Severn, J. R. *Chem. Rev.* **2002, 102,** 3031-3065.

14 12:00 Saturday BSB-117

Reactivity of -ketodiiminate ligands with molybdenum(V) oxidohalides **Y Qi** <*shelly.qi@mail.utoronto.ca*> and **A Hadzovic** <*ahadzovic@utsc.utoronto.ca*>, University of Toronto Scarborough.

Three different -diketiminate ligands (nacnacs; see sheme), were synthesized; and each were reacted with two Mo(V) precursors: green [MoOCl5](pyH)2 and red-brown [MoOBr4](pyH) in acetronitrile with and without base added in an attempt to form mononuclear Mo(V) oxidohalido complexes with these ligands. The reactions proceeded rapidly forming precipitates with colors indicative of diketimine coordination to Mo(V). The presence of base does not seem to influence the reaction outcome or yield. Spectroscopic (IR) and analytical (EA) rsults indicate that only phenyl-substituted nacnac ligand produces a monomeric species cleanly. In other cases the products likely contain polymeric Mo(V) species.



15 09:40 Saturday BSB-121

Stabilizing non-existing RE_4Si_3 and RE_4Ge_3 binaries through the Valence Electron Concentration. **C. Raiju Murugaanandan** <*raijumc@mcmaster*> and **Yurij** <*Mozharivskij*>, Department of Chemistry, McMaster University.

The $RE_4T_{3-x}Pn_x$ (*RE* = Dy, Gd, Ho; T = Ge, Si; Pn = Sb, Bi; x = 0.5 - 3) pseudo binary phases were synthesized to explore the stability of the non-existent RE_4Si_3 and RE_4Ge_3 binaries. Stabilization was achieved through an increase in the valence electron concentration (VEC) via partial pnictogen (Pn) substitutions. The synthesis was performed by arcmelting the starting materials and subsequent annealing in a resistive/induction furnace to attain maximum purity. Powder X-ray analysis was used to establish existence and purity of the binary phases, and Single Crystal X-ray analysis was performed to characterize the crystal structure and determine sample composition.

16 10:00 Saturday BSB-121

Towards the Stable and Surface Active Metal Nanoparticles by the Surface Confined Cross-linking of Ligands **J. K. Yu** <*yu11j@uwindsor.ca*> and **S. Holger Eichhorn** <*eichhorn@uwindsor.ca*>, Department of Chemistry and Biochemistry, University of Windsor, 401 Sunset Avenue, Windsor, Ontario N9B 3P4, Canada.

Organic ligand protected metal nanoparticles (NPs) exhibit different physical and optical properties depending on the type of protection layer. Monolayer coated metal NPs allow functionalization by ligand exchange and potential accessibility to the metal surface but ligand desorption can lead to the destabilization and aggregation of the NPs. In contrast, polymer coated metal NPs provide a high level of protection for the metal surface but its surface accessibility and functionalization is rather limited.

This project aims to design and synthesize a novel organic ligand which provides a stable monomolecular protecting layer combined with an accessibility of the metal surface. The design of this ligand has three components: a flexible anchoring group with a small foot print, a cross-linkable center group (here a tetraol), and a bulky hydrophobic end group. The mismatch of small anchoring group and large end group ensures a loose packing at the surface of the nanoparticles and the tetraol can be cross-linked with, for example, disilanes. Cross-linking of silanes on the surface of gold nanoparticles has recently been demonstrated by the Hegmann group.[1]

1. Mirzaei J, Urbanski M, Kitzerow H.S, and Hegmann T. *Phil. Trans. R. Soc. A*. **2012,***371,* 20120256

17 10:20 Saturday BSB-121

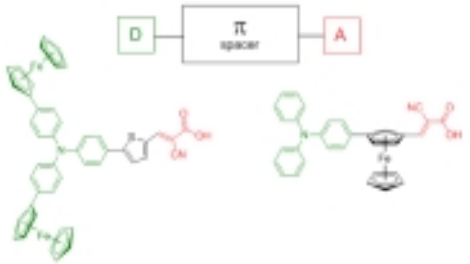
Utilization of bacterial cellulose aerogels as a scaffold for the synthesis of metal oxide catalysts **NW Wisdom** <*nickhugh.wisdom@uoit.net*>, **J Strap** and **L Trevani** <*liliana.trevani@uoit.ca*>, University of Ontario Institute of Technology; **A Vreugdenhil**, Trent University.

Unlike plant based cellulose, bacterial cellulose (BC) has a high degree of purity and crystallinity. The highly ordered tertiary structure consists of microfibrils which are cross-linked via an array of highly ordered hydrogen bonds. These hydrogen bonds impart significant mechanical strength to the cellulose membranes which make them attractive for a wide variety of applications such as artificial arteries, filtration material, fuel cell proton exchange membranes and a myriad of other materials.
The high porosity and specific surface area of cellulose aerogels derived from bacterial cellulose alludes to its applicability as a scaffold for the synthesis of catalyst-polymer composites, particularly metal oxide catalysts using a sol-gel method, because of the abundance of hydroxyl groups and surface adsorbed water. In this study, cellulose aerogels are used as a scaffold for the synthesis of TiO2 nano-rods and tubes, as well as a matrix for the deposition of iron-cobalt mixed oxides. The photocatalytic activity of the synthesized TiO2 particles was assessed by studying the effect on the photodecomposition of methylene blue. Preliminary results are promising and will be presented.

18 11:00 Saturday BSB-121

Novel Ferrocene-containing Dyes for Light Harvesting Applications **N Tulsiram** <*nicholas.tulsiram@ryerson.ca*> and **B Koivisto** <*bryan.koivisto@ryerson.ca*>, Ryerson University.

The low cost dye-sensitized solar cell (DSSC) is the most efficient next-generation photovoltaic cell. The critical component in the cell is the redox active dye molecule, which harvests light and converts it into a photocurrent. This project will focus on incorporating iron-containing dyes into the DSSC by hybridizing ferrocene with existing organic dye scaffolds. Ferrocene has excellent redox stability and is electron-rich and can thus be used as a redox shuttle or a conjugated linker to facilitate the transfer. In addition, substitution on the cyclopentadienyl ring can be used to tune the ferrocene/ferrocenium redox potential, resulting in tuneable dye regeneration rates.



19 11:20 Saturday BSB-121

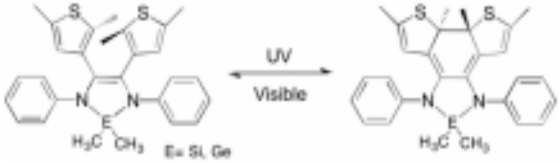
Syntheses and physicochemical properties of ferrocene-BODIPY based dyes <u>**T. Pham**</u> <*tnpham@ryerson.ca*> and **B.D. Koivisto** <*bryan.koivisto@ryerson.ca*>, Ryerson University, Toronto, ON.

Work towards the syntheses and physicochemical properties for a new set of ferrocene-BODIPY based dyes is reported. The combination of a non-innocent π-spacers, such as BODIPY, and the use of a redox active and stable donor, such as ferrocene, facilitates charge separation the excited state, without sacrificing stability and absorption. This is supported by optical and electrochemical experiments in combination with theoretical calculations. These results suggest that energetic tuning of ferrocene may increase the stability of these dyes for light-harvesting applications.

20 11:40 Saturday BSB-121

Synthesis and photochromism of a silicon and germanium substituted dithienylethene ligand. <u>**A Evans**</u> <*aevans48@uwo.ca*>, **J.T. Price** <*jprice6@uwo.ca*> and **P.J. Ragogna** <*pragogna@uwo.ca*>, Department of Chemistry and the Center for Materials and Biomaterials Research, Western University, 1151 Richmond St, London, Ontario, N6A 5B7.

Photochromic dithienylethenes have been widely studied given their potentially useful application in optoelectronics as rewritable devices and molecular switches.[1] These molecules can be functionalized in order to alter their photophysical properties while maintaining high fatigue resistance and thermal irreversibility.[1] In this context, we have designed a diazabutadiene functionalized DTE ligand with the potential to coordinate to transition metals, lanthanides and other main group elements while maintaining the desired photochromic properties. The successful incorporation of group 14 elements (silicon and germanium) was achieved, and as targeted, the desired ring closing and opening reactivity was maintained.The synthesis of these complexes and their photochromic properties will be discussed.



(1) Irie, M. *Chem. Rev.* **2000**, 100, 1685-1716.

21 12:00 Saturday BSB-121

Electron Spin Resonance Studies on the Dimerization of 1,2,3,5-Dithiadiazolyl Radicals <u>**J.M Mohamud**</u> <*mohamudj@uwindsor.ca*>, **J.M Rawson** <*jmrawson@uwindsor.ca*> and **J Hayward** <*jhayward@uwindsor.ca*>, University of Windsor.

Electron Spin Resonance Studies on the Dimerization of 1,2,3,5-Dithiadiazolyl Radicals

The use of P-block elements in our group has lead to the synthesis of a number of different Sulfur Nitrogen heterocyclic compounds that are capable of forming stable radical monomers at room temperature. These radicals possess a single unpaired electron, allowing them to display paramagnetic behavior, giving them numerous potential applications in the field of applied electronics as organic molecular magnetic switches. The main area of concern though is that while the monomeric radical form is of great interest, it is capable of undergoing a dimerization process with other radical monomers to form the diamagnetic dimer, which possesses no unpaired electrons. Electron Paramagnetic Resonance (EPR) spectroscopy is a valuable tool to examine the dimerization process, because the spectrometer depends on the presence of unpaired electrons in order to observe an absorption profile, meaning the monomeric species is EPR active, while the dimeric species is EPR silent. Furthermore, previous studies have shown that the dimeric species is favoured in low temperatures, while the monomer is favored at room temperature. Using variable temperature studies, we can experimentally determine the thermodynamic values associated with the dimerization process. While studies have been carried out for different dithiadiazolyl radicals, these have been examined for solid state samples, or a singular solvent. The purpose of this project is to examine the dimerization of dithiadiazolyl radicals in solution, using a gradient of

22 09:40 Saturday BSB-136

Immunological detection of cytochrome b5 isoform I in Giardia lamblia <u>**M Teghtmeyer**</u> <*meganteghtey@trentu.ca*> and **S Rafferty** <*srafferty@trentu.ca*>, Trent University.

Giardia lamblia is a protozoan intestinal parasite which is found across the globe and is particularly a problem in poverty-stricken regions due to drinking contaminated water. It is a highly divergent eukaryote that lacks mitochondria, a respiratory chain and common heme proteins such as respiratory chain cytochromes and catalase. Giardia also lacks the enzymes for heme biosynthesis. In spite of this Giardia has genes for at least four heme proteins, one flavohemoglobin and three isoforms of cytochrome b5. Cytochrome b5's are a superfamily of small ubiquitous heme-binding proteins which are used for electron transfer mediation between different proteins. The three Giardia cytochrome b5 isoforms are isolated as heme-containing proteins when expressed in E. coli, but the presence of these proteins has not been confirmed. To determine in vivo expression of cytochrome b5 a Western blotting technique was used with an antibody raised against Giardia cytochrome b5 isotype I (gCYTB5-I). This antibody reacts specifically with recombinant gCYTB5-I and will not react with the other two isotypes. Using this technique we have determined that Giardia trophozoites expresses gCYTB5-I.

23 10:00 Saturday BSB-136

Ubisol QE as a preventative treatment for MPTP induced neurodegeneration in DJ-1 deficient genetically susceptible mice model of Parkinson's disease <u>**H. Jasra**</u> <*jasrah@uwindsor.ca*>, **K. Muthukumaran** <*muthuku@uwindsor.ca*>, **J. Smith** <*smith12q@uwindsor.ca*>, **J. Cohen** <*jcohen@uwindsor.ca*>, **D. Lopatin** <*lopatin@uwindsor.ca*> and **S. Pandey** <*spandey@uwindsor.ca*>, University Of Windsor, Sunset Ave., Windsor, ON, N9B 3P4; **M. Sikorska** <*Marianna.Sikorska@nrc-cnrc.gc.ca*> and **J. Sandhu** <*jagdeep.Sandhu@nrc-cnrc.gc.ca*>, National Research Council Canada, Montreal Rd., Ottawa, ON, K1A 0R6.

Parkinson's disease (PD) is the second most common neurodegenerative motor disorder caused by a lack of dopamine due to the death of dopaminergic neurons in the substantia nigra region of the brain. Recent research suggests that most cases of PD arise as a result of a combination of environmental and genetic risk factors. Loss-of-function mutations in many genes have been identified and well validated to show an increase in the susceptibility of PD, among them is the DJ-1 gene. Though the true cause of PD is still unclear, certain toxic agents are known to cause neurodegeneration, such as paraquat and MPTP. We work with a water soluble formulation of CoQ10 (Ubisol QE) and have shown that it is effective in protecting neurons in the environmental toxin induced rat model of PD. In this study we combine DJ-1 deficiency and MPTP toxicity to create a more representative model of PD, one of genetic susceptibility. We have shown that Ubisol-QE is able to prevent neurodegeneration of dopaminergic neurons as a prophylactic treatment in DJ-1 deficient mice. Also, the DJ-1 mutation does increase the susceptibility to neurodegeneration when exposed to the neurotoxin MPTP in comparison to the corresponding wild type. These results are indispensable to the search for a preventative therapy for people genetically predisposed to develop PD.

24 10:20 Saturday BSB-136

Targeting Mitochondrial and Oxidative Vulnerabilities Using Synthetic Analogues of Pancratistatin in Breast Cancer <u>**S Joshi**</u> <*joshif@uwindsor.ca*>, **D Ma**, **D Tarade** and **S Pandey** <*spandey@uwindsor.ca*>, Department of Chemistry and Biochemistry, University of Windsor, 401 Sunset Avenue, Windsor, Ontario N9B 3P4, Canada; **S Vshyvenko** and **T Hudlicky**, Chemistry Department and Centre for Biotechnology, Brock University, 500 Glenridge Avenue, St. Catharines, Ontario L2S 3A1, Canada.

Cancer cells have a distinct metabolic phenotype, depending less on mitochondria and more on glycolysis for energy. This glycolytic shift and mitochondrial remodelling confers a proliferative advantage and an acquired resistance to apoptosis. Cancer cells also possess high basal levels of reactive oxygen species (ROS) and are predicted to be more dependent on cellular stress response mechanisms to ROS than normal cells. We found that the natural compound pancratistatin (PST) and synthetic analogues induce apoptosis in breast cancer cells in 2D and 3D culture specifically by mitochondrial targeting as they were shown to cause mitochondrial membrane potential collapse. Moreover, when treated with isolated cancer cell mitochondria, they increased production of ROS. N-acetylcysteine, an antioxidant, was able to rescue breast cancer cells from PST and PST-induced cell death indicating that ROS production is essential to the toxicity of these compounds. Notably, PST and its analogues were more effective against breast cancer cells than the commonly used chemotherapeutics taxol and tamoxifen. Hence, we present novel strategies targeting mitochondrial and oxidative vulnerabilities in cancer cells with PST analogues and other low toxic agents as potentially safe and effective alternatives to current cancer therapies.

25 11:00 Saturday BSB-136

Seeking the redox partners of *Giardia lamblia* cytochrome b_5 **K. Campanaro**, **S. Rafferty** and **J. Yee**, Trent University.

The biochemistry of waterborne protozoan parasite *Giardia lamblia* is intriguing. Without mitochondria it lacks the ability to make heme or to require this cofactor for respiratory cytochromes. Yet the Giardia genome does encode heme-binding proteins, including flavohemoglobin and three isoforms of the cytochrome b_5 family, all of which have been expressed as recombinant proteins with heme bound to them. The roles of cytochrome b_5 in Giardia and their redox partners are unknown. However, many electron donors to known cytochromes b_5 are enzymes that use nicotinamide cofactors as an electron source. My research used UV-visible spectroscopy to screen Giardia cell lysates for NAD(P)H oxidase activity that is stimulated by recombinant Giardia cytochrome b_5 isotype I (gCYTb5-I). Stimulation of NAD(P)H is observed under both aerobic and anaerobic conditions, yet gCYTb5-I remains in its oxidized form. Future research to further investigate the electron transport partners of cytochrome b_5 needs to be conducted in order to gain clues as to why cytochromes b_5 are present in this unique parasite.

26 11:20 Saturday BSB-136

Evaluating the Anti-Cancer Activity of Synthetic Analogues of Pancratistatin in Colorectal Cancer and Leukemia Cells and in Colon Tumor Xenografts **J Church** <*churchj@uwindsor.ca*>, **D Ma**, **K Stokes** and **S Pandey** <*spandey@uwindsor.ca*>, Department of Chemistry and Biochemistry, University of Windsor, 401 Sunset Avenue, Windsor, Ontario N9B 3P4, Canada; **S Vshyvenko** and **T Hudlicky**, Chemistry Department and Centre for Biotechnology, Brock University, 500 Glenridge Avenue, St. Catharines, Ontario L2S 3A1, Canada.

The current treatments of cancer include surgery, radiation therapy, and chemotherapy. However, many chemotherapeutics are unspecific to cancer cells and have adverse effects. We have found that the natural compound Pancratistatin (PST) specifically induces apoptosis in cancer cells by mitochondrial targeting. However, preclinical and clinical work has been hindered by its low availability in nature. To overcome this, we synthesized and screened numerous analogues of PST for anti-cancer activity. We discovered some of these analogues have comparable or superior anti-cancer activity, specifically inducing apoptosis in leukemia, and colorectal cancer cells by mitochondria targeting; isolated cancer cell mitochondria treated with these analogues showed an increased production of reactive oxygen species and release of apoptogenic factors. Furthermore, these PST analogues were able to reduce growth of human p53 positive and negative colon tumours in immunocompromised mice. Importantly, these analogues exhibited minimal toxicity in mice as well as in various noncancerous colon cell lines and normal leukocytes from healthy volunteers. Therefore, PST analogues may serve as a safe and potent alternatives to current chemotherapeutics by targeting cancer cell mitochondria.

27 11:40 Saturday BSB-136

Characterization of cells with unusually high DNA content in the Giardia lamblia trophozoite cell cycle

The waterborne protozoan parasite Giardia lamblia is found worldwide and causes the diarrheal disease known as giardiasis. The parasite is found in two forms, the infectious cyst and the motile trophozoite. During the cell cycle, trophozoites at the G1 stage are tetraploid with a total DNA content of 4N, and trophozoites at the G2 stage are octoploid with a total DNA content of 8N. However, we also detected a small percentage of cells that have a DNA content of 16N in these cultures, and their appearance is induced by the addition of drugs that perturb the cell cycle. Our hypothesis is that the 16N cells represent a pre-encystation stage of Giardia that is induced by cellular stress. Counterflow centrifugal elutriation was used to obtain fractions of Giardia cultures enriched in the 16N cells for microscopic analysis. We also used quantitative RT-PCR to examine the expression of genes that are expected to be induced by stress or by encystation in these samples. These results and their significance will be discussed in the presentation.

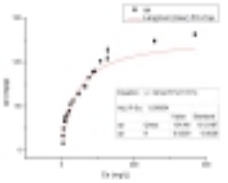
28 12:00 Saturday BSB-136

Elucidating the Structure and Function of Streptomyces hawaiiensis ClpP proteases **P. K. Patel** <*patelpk3@mcmaster.ca*> and **J. Ortega** <*ortegaj@mcmaster.ca*>, McMaster University.

Proteases play a vital function in maintaining protein homeostasis. One such key protease that is present in most bacterial species is caseinolytic protease P (ClpP), which mediates the degradation of proteins in bacteria. It requires the association of ATPases in order to degrade substrates. A new class of antibiotics, the acyldepsipeptide (ADEP) molecule, binds to ClpP and activates the protease independently from the ATPases, which results in unregulated degradation of polypeptides in bacterial cells, eventually leading to bacterial cell death. ADEP is produced by Streptomyces hawaiiensis, whose genome contains clpP genes. Previous studies of ClpP in E. coli, B. subtilis and other bacterial species have indicated that the bacteria die in the presence of ADEP. However, it is uncertain as to how S. hawaiiensis is able to survive the deleterious effects of ADEP. In this research study, the structure and functions of the ClpP proteases of S. hawaiiensis are explored. The proteins were selectively expressed in plasmids, grown and then purified using column chromatography. The proteins were then subjected to various in vitro activity assays to decipher their proteolytic activity. Functional activity assays for three of the ClpP proteases, ClpP-ADEP, ClpP1 and ClpP2 was performed and ClpP1ClpP2 combination was found to be highly active in the presence of ADEP. The proteins were also visualized using negative staining electron microscopy to obtain a projection structure of the proteases. Structurally, it is concluded that ClpP1 and ClpP2 assemble in a similar yet a different tetradecameric complex than those studied in other bacterial species. The mode of resistance of S. hawaiiensis against this antibiotic is hypothesized to be due one of its key ClpP proteases, ClpP-ADEP, which is yet to be tested using dynamic light scattering technique and competition assays.

29 09:40 Saturday BSB-138

SOYBEAN PEROXIDASE IMMOBILIZATION ON ORTHO-CRESOL POLYMERIC SOLIDS, AN AID TO ENZYME PRODUCTION **Y. Xiao** <*xiao8@uwindsor.ca*> and **W. Feng**, Environmental Chemistry Lab, Univeristy of WIndsor, 401 Sunset Avenue.



Soybean Peroxidase (SBP) works well in the enzymatic treatment of phenolic waste water to form a polymeric solid. A major issue in enzyme production is concentrating it from a dilute extract. The polymeric solids from enzymatic treatment of phenol might play a special role in the concentrating process, by immobilizing the enzyme, thence allowing its elution in the presence of the non-ionic surfactant, Triton X-100 (Triton). Earlier work in this lab has shown that SBP and Triton have shown competitive adsorption on poly-phenol solids. In our research, o-cresol, a more hydrophobic substrate, was studied, first to determine the optimum values of SBP and Triton concentration for > 95% removal of 1 mM o-cresol in 3 h: without Triton, 0.8 U/mL SBP was needed; in presence of 60 mg/L Triton, 0.02 U/mL SBP was needed. SBP adsorption on o-cresol solids follows a Langmuir isotherm with maximum capacity 1.84 U/mL and half-saturation concentration at 0.10 U/mL. For Triton, between 0 and 400 mg/L equilibrium concentrations, the adsorption pattern followed a Langmuir isotherm with maximum capacity 154 mg/g and half- saturation concentration at 41.8 mg/L. Also, Triton's adsorption beyond a monolayer follows a BET isotherm. The final goal is to develop a reproducible protocol for concentrating SBP using o-cresol solids.

30 10:00 Saturday BSB-138

Design of a Tool for Photocontrol of Translation **R Ariyakumaran**, **A Kumar**, **A.S.I. Jaikaran** and **G. Woolley**, University of Toronto.

Local translation in the axons and dendrites of neurons has recently been shown to be important in neurological development. A tool to control local translation in different areas of developing neurons could be important for understanding the biochemistry of this developmental process. Eukaryotic translation initiation requires the formation of the eukaryotic initiation factor-4F (eIF4F) complex which is made of three subunits eIF4E, eIF4A and eIF4G. This complex binds to the 5'cap of mRNAs and facilitates the loading of ribosomal subunits onto the mRNA. This process, called cap-dependent translation initiation, is regulated by the association and dissociation of 4EBP (eIF4E-binding protein) via competitive binding with eIF4G.

Here, we report designs and characterization of photoswitchable eIF4E-binding proteins in which segments of the 4EBP sequence are fused with known photoswitchable protein scaffolds. The scaffolds used include a circularly permutated photoactive yellow protein, a modified version of a soluble protein from Halorhodospira halophila, a LOV2 domain, a relatively small blue light sensitive protein from Avena sativa phototropin, and a circular permuted LOV2 domain. The designed proteins are highly soluble and well folded when overexpressed in E. coli under dark conditions, and undergo PYP-like and LOV-like photocycles respectively upon irradiation of blue light. The thermal relaxation of the protein to the dark-adapted state after irradiation varies considerably between the designed constructs. UV-Vis absorption data indicate that cPYP based 4EBPs recover more slowly (minutes) than the LOV based chimeras (seconds). Fluorescence-monitored GdnMHCl denaturation experiments and temperature

31 10:20 Saturday BSB-138

Exploring The Silicon Substrate Tolerance of the Diatom *Nitzschia curvilineata* **J.L. DeJong** and **P.M. Zelisko*** <*pzelisko@brocku.ca*>, Dept. of Chemistry, Brock University.

It is of interest to develop a biotechnological process that would permit biocatalysis at or near silicon atoms. Although there are numerous terrestrial and aquatic species that naturally perform chemistry at silicon atoms, diatoms are perhaps the most widely studied This research seeks to examine the silicate substrate tolerance of the diatom species *Nitzschia curvilineata*. The diatoms were challenged with methyltrimethoxysilane in place of the natural substrate sodium silicate to observe the effect of the methyl group on the diatom population. The findings indicated that although *Nitzschia curvilineata* do continue to live and replicate under the altered environmental conditions, chlorophyll A and turbidity measurements demonstrated that the growth rates of the populations exposed to methyltrimethoxysilane were slower than that of the populations exposed to sodium silicate. Optical and scanning electron microscopy imaging of the diatom samples, however, did not demonstrate any gross morphological differences relative to that of the controls.

32 11:00 Saturday BSB-138

Isolation and Characterization of Catalytic DNA via Independent *In Vitro* Selection **RE Gysbers** <*gysberre@mcmaster.ca*>, **K Tram** <*tramkq@mcmaster.ca*> and **Y Li** <*liying@mcmaster.ca*>, McMaster University.

Many disciplines of science, from medical therapeutics to analytical biosensors, have been impacted by the discovery of functional nucleic acids such ribozymes and deoxyribozymes. The process of *in vitro* selection, involving the isolation of a catalytically active molecule from a large random library, has been performed multiple times to obtain both types of these functional nucleic acids. Through selective pressures and enrichment, *in vitro* selection is capable of evolving a functional catalyst in the absence of structural knowledge as well as enriching the catalyst through mutation. In the case of deoxyribozymes, several motifs have emerged; the most characterized DNAzyme motifs capable of RNA cleavage are 8-17 and 10-23. Multiple independent selection procedures have led to the isolation of an assortment of variants of 8-17, which is known as the simplest RNA-cleaving motif. The objective of this project is to obtain and enrich DNAzymes from two different random libraries of differing sequence length; the DNA sequence will be selected for its ability to cleave an RNA site. The characterization of the products of these two parallel but independent *in vitro* selection experiments will then be performed.

33 11:20 Saturday BSB-138

Novel approach to detect *Listeria monocytogenes* **Q. Feng** <*fengq4@mcmaster.ca*>, **P. Kanda** <*kandap@mcmaster.ca*> and **Y. Li** <*liying@mcmaster.ca*>, McMaster University,, Hamilton ON, L8S 4L8.

Foodborne pathogens such as *Listeria monocytogenes* pose serious threats to public health and safety as seen from the 2008 outbreak in Maple Leafs Food. Such outbreaks question the validity and standards of quality control necessary to prevent future occurrences. While current detection methods are often time-consuming and expensive, alternative technologies that are portable, accurate, and cost-effective need to be developed. A novel method to improve current regime of pathogen detection involves aptamers, which are small single-stranded DNA or RNA molecules with the ability to bind a specific target of interest. We have designed aptamers, which will be selected using *in vitro* selection in the test tube, to specifically recognize and bind to an endoribonuclease (RNase) from *L. monocytogenes* for bacterial detection. This aptamer probe not only binds RNase but also contains a single ribonucleotide within its sequence that can be hydrolysed by the RNase enzyme. The clever placement of a fluorophore and quencher pair on the aptamer probe allows the RNA hydrolysis event to be visualized by fluorescence (see Figure). Thus far, I have been working towards cloning and purification of RNase Y from *L. monocytogenes*, which will be used as the target for the aptamer probe. We are also working towards the development of aptamers which target other RNases, such as RNase G, RNase III, and RNase HII.

34 11:40 Saturday BSB-138

Efficient Methods in Creating Hemoglobin Based Blood Substitutes **A Wang** <*aizhou.wang@mail.utoronto.ca*> and **R Kluger** <*rkluger@chem.utoronto.ca*>, Department of Chemistry, University of Toronto, 80 St. George Street , Toronto, ON, M5S 3H6.

The use of stabilized tetrameric hemoglobin as an alternative to red cells in blood transfusions has revealed significant increases in blood pressure in clinical trials. This has been attributed to the scavenging of nitric oxide by extravasation. A high molecular weight cross-linked hemoglobin bistetramer, produced by CuACC between a bis-alkyne linker and azide-functionalized crosslinked hemoglobin, appears to be a potent red cell substitute with appropriate oxygenation properties. However, all reported methods of introducing the azide moiety give heterogeneous products, some of which do not lead to the desired bistetramer. This not only wastes the protein that is unreactive but also makes separation of proteins necessary, which is slow, costly, and inefficient. In order to improve the efficiency of this reaction, methods to eliminate the unreactive - crosslinked species in early stages are exploited. In particular, the accessibility of the desired site (β-Lys82) was strategically increased by making the undesired site (α-Lys90) unreactive via site-specific aminolysis using a 3,5-dibromosalicylate ester as the acylating agent. The potency of the α-site acylation revealed much more specific cross-linking. The resultant α-acetylated crosslinked hemoglobin azide was able to produce bistetramer using the CuACC method. CD spectroscopy of the modified species showed little change to the tertiary structure of the hemoglobin despite the chemical intervention. Thus, the α-specific acylation is a potentially viable method for the efficient production of a hemoglobin based blood substitute.

35 12:00 Saturday BSB-138

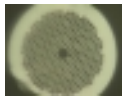
Biochemical characterization of a novel MLH1 missense variant in the diagnosis of HNPCC **A. Zhou** <*zhoua4@mcmaster.ca*> and **A. Guarne** <*guarnea@mcmaster.ca*>, McMaster University, 1280 Main Street W., Hamilton, ON; **K. Bell** <*kathleen.bell@jcc.hhsc.ca*> and **K. Zbuk** <*kevin.zbuk@jcc.hhsc.ca*>, Juravinski Cancer Centre, McMaster University, 699 Concession Street, Hamilton, ON.

Hereditary non-polyposis colorectal cancer (HNPCC) is the most common form of hereditary colorectal cancer (CRC). Mutations in the *msh2* and *mlh1* genes account for greater than 90% of germline mutations in HNPCC. The MSH2-MSH6 and MLH1-PMS2 heterodimers are critical to the initiation of DNA Mismatch Repair (MMR), a highly conserved process that maintains genome stability by correction of DNA replication errors. The challenge of classifying novel mutations found in MMR genes as pathogenic HNPCC mutations presents a barrier to the implementation of preventative programs. Using structural modeling, molecular cloning and protein biochemistry, we have characterized a novel mutation, C680R in MLH1, found in the individuals of a suspected HNPCC family. Modeling on the MLH1 crystal structure suggested that the mutation would disrupt the folding around a tight hydrophobic pocket. Its introduction into a stable construct of the MLH1 dimerization domain resulted in insoluble protein, presumably due to unfolding. PMS2 is unable to fold correctly in the absence of correctly folded MLH1, and accordingly, both MLH1 and PMS2 deficiency was observed in the tumours of patients carrying the mutation. This confirmed the folding defect in the MLH1-C680R variant and resultant loss of MMR function in these individuals. Our work contributed to the classification of the C680R mutation in MLH1 as a pathogenic MMR missense mutation and demonstrates the utility of biochemical characterization of unclassified variants to clinical diagnoses of HNPCC.

36 09:40 Saturday BSB-137

Microanalytical Separation in a Photonic Crystal Fiber **N. Gibson** <*8nag1@queensu.ca*> and **P. Loock** <*peter.loock@chem.queensu.ca*>, Chemistry Department, Queen's University.

In liquid chromatography, packed columns are used much more frequently than open tubular columns even though the latter can theoretically provide higher resolution. This is due to the low diffusion coefficients in liquids, which imposes a restriction on the size of an open column to a diameter of a few microns. A single OTLC column would therefore have a limited loading capacity and high flow resistance. A photonic crystal fiber, conventionally used as an optical waveguide, is employed as a multi-channel OTLC column to increase the capacity and lower the resistance. An inherent outcome of the manufacturing process of PCFs poses a large issue for their use in separations, and that is the variance in channel diameter. To compensate for the differences in channel size, a flow reversal technique is applied to refocus the analyte bands. Single analyte refocusing has been demonstrated to attest to the application of the flow reversal technique, and a separation will be carried out in the near future. One solvent can be used in the refocusing of a single analyte, but a different solvent must be used in the reverse direction when performing a separation.



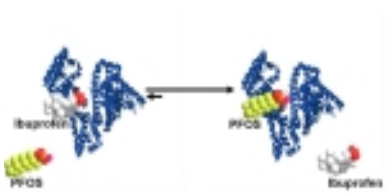
37 10:00 Saturday BSB-137

The Effects of Low Molecular Weight Organic Acids on the Desorption of Lead from Natural Soils **C.A. Cheyne** <*carol.cheyne@mail.utoronto.ca*> and **J.G. Murphy** <*jmurphy@chem.utoronto.ca*>, Department of Chemistry, University of Toronto.

The treatment of metal-contaminated soils using low molecular weight organic acids (LMWOAs) has been proposed as a low-cost remediation technique. Three LMWOAs were analyzed for their ability to desorb and mobilize lead in natural soil samples collected in Egbert, Ontario. Soil samples were spiked with lead and atomic absorption spectroscopy was used to compare lead levels in control solutions and those treated with LMWOAs. Acetic acid, glutaric acid, citric acid, and an electrolyte were used to evaluate the effects of pKa and molecular structure on the desorption process at a range of pH values. Citric acid was superior in lead desorption, while acetic and glutaric acid were only marginally more effective than the electrolyte. Acidic conditions made desorption favourable, yet citric acid was most successful between pH 5.5 and 6, when it is doubly deprotonated. Additionally, desorption solutions were analyzed by ion chromatography to assess the effects of applied LMWOAs on calcium and magnesium concentrations in the soil. It was shown that at each LMWOA's optimal pH for lead desorption, a significant amount of calcium and magnesium was also mobilized. It was concluded that citric acid may be effective in assisting in soil remediation, either by phytoremediation or electrokinetic remediation. However, since the applied LMWOAs also desorb essential minerals, this method should only be applied on soils used in construction or landfill cover, and should not be used in ecologically important soils.

38 10:20 Saturday BSB-137

Competitive Binding of Ibuprofen and Perfluoroctanesulfonic Acid with Serum Albumin Studied by Electrospray Ionization Mass Spectrometry **ML D'Alessandro** <*michelledales@trentu.ca*>, **DA Ellis** <*davidellis@trentu.ca*> and **RE March** <*rmarch1@cogeco.ca*>, Trent University , Department of Chemistry, 1600 West Bank Drive, Peterborough, Ontario, K9J7B8.



Serum albumin reversibly binds and transports endogenous and exogenous ligands, such as pharmaceuticals whose therapeutic efficacy is dictated by liberation from the protein. Aqueous perfluoroctanesulfonic acid (PFOS) is a bioaccumulative, pervasive species of anthropogenic origin found in the serum of 90% of Americans that binds with high affinity to serum albumin in the same specific location as pharmaceuticals such as ibuprofen. Therefore, competitive protein binding between PFOS and ibuprofen has the potential to alter the pharmacological activity of the drug. Using electrospray ionization mass spectrometry, the competitive interaction between ibuprofen and PFOS has been investigated. It is demonstrated that PFOS will displace all bound ibuprofen molecules from serum albumin and prevent further binding of the drug when the fluorinated analyte concentration exceeds half that of ibuprofen. These observations suggest that PFOS may displace ibuprofen and pharmaceuticals of similar binding location in the body under physiological conditions thus altering the pharmacokinetics, toxicity, and deposition of such drugs.

39 11:00 Saturday BSB-137

Towards the development of a Sequencer-On-A-Chip for in-field Species Identification: On-Chip Isothermal Amplification of DNA Barcodes **B.N. Udugama** <*buddhisha.udugama@mail.utoronto.ca*>, **M.S. Gams** <*miki.gams@mail.utoronto.ca*>, **R.N. Bialy** <*roger.bialy@mail.utoronto.ca*>, **W.A. Otieno** <*wendy.otieno@mail.utoronto.ca*>, **P. Piunno** <*paul.piunno@utoronto.ca*>, **S. Stefanovic** <*sasa.stefanovic@utoronto.ca*>, **U.J. Krull** <*ulrich.krull@utoronto.ca*> and **V. Barzda** <*virgis.barzda@utoronto.ca*>, University of Toronto Mississauga.

Development of a portable DNA-sequencer capable of sample preparation, amplification, and sequence determination represents a growing field of research; particularly for real-time species identification in applications such as food authenticity testing. Species identification was based on DNA barcodes, which requires amplification of mitochondrial cytochrome C oxidase 1 (CO1) DNA. Thermophilic helicase-dependent amplification (tHDA), which closely mimics *in vivo* DNA replication, was selected for incorporation into the portable sequencer. This isothermal method offers fast results (90 min) and provides for simplified microchip design with respect to PCR. Amplification of the CO1 region by tHDA for species identification and subsequent miniaturization of this technique has not been previously investigated.
Our study investigated the suitability of tHDA for species identification in typical reaction vials on the macroscopic scale as well as on a miniaturized platform. tHDA was used to amplify a 100bp region of the CO1 gene in G*romphadorhina portentosa*. Work done on primer design and assay optimisation will be discussed, in addition to our progress toward achieving on-chip amplification.

40 11:20 Saturday BSB-137

Towards the development of a Sequencer-On-A-Chip for in-field Species Identification; Optimization of Sieving Matrix Formulations for On-Chip Sanger Sequencing. **R.M. Bialy** <*roger.bialy@mail.utoronto.ca*>, **M.S. Gams** <*miki.gams@mail.utoronto.ca*>, **W.A. Otieno** <*wendy.otieno@mail.utoronto.ca*>, **B.N. Udugama** <*buddhisha.udugama@mail.utoronto.ca*>, **V. Barzda** <*virgis.barzda@utoronto.ca*>, **U.J. Krull** <*ulrich.krull@utoronto.ca*>, **P.A.E. Piunno** <*paul.piunno@utoronto.ca*> and **S. Stefanovic** <*sasa.stefanovic@utoronto.ca*>, University of Toronto at Mississauga, Dept. Chem. Phys. Sci and Dept. Biol.

There is significant interest in the development of a field-portable DNA barcoder for rapid species identification, particularly with regards to application in food authenticity testing and for identification of invasive species. The device should be capable of nucleic acid extraction, followed by amplification of the Cytochrome-C Oxidase Subunit 1 (CO1) mitochondrial DNA barcode sequence, and sequence determination. The sequence of the first 100-200 bases of CO1 can then be compared to the Barcode of Life database and the species of the sample determined.

This presentation will focus on the optimization of the sequencing portion of the device. The well-established Sanger method of DNA sequencing has been implemented, which requires electrophoretic separation of fluorescently tagged DNA sequences of various lengths with single nucleotide resolution. This will be achieved by inclusion of a micro channel electrophoresis component, which will be optimized to achieve the desired resolution in the smallest form-factor possible. A two-level factorial design for the optimization of both the sieving matrix and the buffer solution will be discussed.

41 11:40 Saturday BSB-137

Investigating the folding intermediates of Cytochrome c using Traveling Wave Ion Mobility Mass Spectrometry **S. Hakimzadah** <*shakhak@yorku.ca*>, York University, 4700 Keele St. West, Toronto, ON, M3J 1P3.

Proteins must fold into their specific 'native' structure to carry out their function. During this process, proteins spontaneously follow distinct step-wise folding pathway thereby occupying characteristic folding intermediates. However, certain intermediates can reflect an incorrect refolding pathway of proteins that may lead to aggregation, which is associated with neurodegenerative disease. Using a Waters Synapt G1 Ion-mobility mass spectrometer, Cytochrome c intermediates were observed by Electrospray Ionization Mass Spectrometry (ESI-MS) to look at protein unfolding in acetic acid. The use of ion mobility allowed for separation of co-populated cyt c intermediates with the same charge-state. The population of folded or partially folded intermediates from kinetic and equilibrium mode were then compared based on their drift time distributions. Drift times for the intermediates were the same, which suggests that the equilibrium and kinetic intermediates are structurally similar to one another.

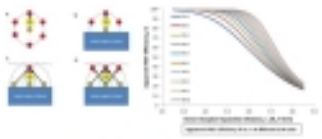
42 12:00 Saturday BSB-137

Measuring the Dynamics of Schizosaccharomyces pombe La in the Absence and Presence of RNA, Using Time Resolved Mass Spectrometry and Microfluidics Enabled H/D Exchange. **A Shaikh** <*aasefa11@yorku.ca*> and **D.K. Wilson**, York University.

Schizosaccharomyces pombe La (sLa1) protein binds to the 3' end of RNAs and protects it from degradation caused by exo-nucleases, allowing it to mature and associate with proteins to form functional RNA-protein complexes. While the RNA targets of sLa1 have been well characterized, the nature of the binding interaction is not well understood. This project focusses on understanding the changes in dynamics that accompany RNA binding in sLa1. The dynamics of the protein as it fluctuates between unfolded and folded conformers in the absence and presence of RNA was studied on a millisecond time frame using bottom-up time resolved mass spectrometry. Subsequently, hydrogen-deuterium exchange using a microfluidic chip was employed to study the amount of exchange between the backbone amide hydrogen and deuterium in the absence and presence of RNA. Our findings indicate that in the absence of RNA, sLa1 is largely unfolded, whereas in the presence of RNA, the protein achieves an equilibrium in which both the unfolded and unfolded conformers are present. Moreover, a higher amount of exchange is seen for backbone amide hydrogen and deuterium in the absence of RNA, than in the presence of RNA. In the presence of RNA, regions were identified with lower levels of exchange compared to RNA-free, suggesting a binding epitope.

43 09:40 Saturday BSB-115

Theoretical Modeling: For an Interfacial Fluorescence Resonance Energy Transfer in Quantum Dot Donor - Dye Acceptor Biorecognition System **K. Wan** <*justin.wan@mail.utoronto.ca*> and **U.J. Krull** <*ulrich.krull@utoronto.ca*>, Chemical Sensor Group,, University of Toronto Mississauga,, 3359 Mississauga Road N., Mississauga, ON L5L 1C6.



In the field of bioanalytical chemistry, fluorescence resonance energy transfer (FRET) is widely used as a method to detect a target (FRET acceptor) when it is in close proximity to an energy donor. Recently, solid-phase bioassays have been developed using colloidal nanoparticles (quantum dots, QDs) as FRET donors, with conjugated oligonucleotide probes as sites for capture of dye-labeled oligonucleotides (acceptors). Solid-phase assays that immobilized QDs donors in a dense layer onto silica and plastic surfaces showed significant FRET signal enhancement when compared to equivalent quantities of the FRET pairs in bulk solution. Such an enhancement is a novel feature offering analytical advantage in bioassay design. A novel model will be presented that explores interfacial FRET using layers of QDs and acceptors. Probability functions of energy transfer suggest that the FRET efficiency in two-dimensions is dependent on the donor-acceptor ratio as well as the fluorescence lifetimes of the donors and the acceptors. Experimental work has been performed to test the model, and makes use of control of the donor-acceptor ratio on a solid support via construction of one-donor-one-acceptor conjugates.

44 10:00 Saturday BSB-115

Path integral simulations of hydrogen molecules trapped in water clathrate cages **J. T. Cantin** <*jtcantin@uwaterloo.ca*>, **T. Zeng** <*tzeng@ualberta.ca*>, **M. Schmidt** <*mdgschmi@uwaterloo.ca*> and **P.-N. Roy** <*pnroy@uwaterloo.ca*>, Department of Chemistry, University of Waterloo, Waterloo, Ontario N2L 3G1, Canada.

Hydrogen clathrate hydrates where hydrogen molecules are trapped in nanoscale cages of water molecules are of interest as potential candidates for energy storage materials. A significant amount of both experimental and theoretical work has been reported in the literature that has tried to both evaluate the suitability of hydrogen clathrate hydrate for hydrogen storage purposes and to understand its underlying mechanisms. The theoretical work has generally treated the cages classically, while the hydrogen molecules have generally been treated quantum mechanically and within a rigid cage. The present work intends to expand upon this previous research by using path integral methods in order to investigate the cage dynamics quantum mechanically, treat the hydrogen molecules within a rigid cage with an adiabatic hindered rotor approximation, and then combine the two methods in order to treat hydrogen molecules within a flexible cage quantum mechanically. Specifically, the heat capacities involved, the presence of any guest-host coupling, and ortho-para conversion of the hydrogen molecules within the clathrate are to be investigated. By further understanding the underlying processes that drive the properties and stability of the hydrogen clathrate hydrate, better hydrogen storage materials could be designed.

45 10:20 Saturday BSB-115

Accelerating quantum molecular dynamics simulations using graphical processing units **K Bishop** <*kpbishop@uwaterloo.ca*>, **N Faruk** <*nffaruk@gmail.com*>, **M Schmidt** <*mdgschmi@uwaterloo.ca*> and **P.-N. Roy** <*pnroy@uwaterloo.ca*>, University of Waterloo.

Graphical Processing Units (GPUs) can be used to accelerate Path Integral Molecular Dynamics (PIMD). We prepared an installation guide to allow other users to install the Molecular Modelling Toolkit (MMTK) and Open Molecular Mechanics (OpenMM). This software allows for the execution of PIMD simulations on a variety of platforms. In order to test the performance of our implementation, various cluster systems consisting of argon, neon, and parahydrogen particles have been simulated using a new implementation of PIMD. We have focused on the use of tabulated potentials in order to treat a wider variety of systems. The GPU implementation via OpenMM decreases the execution time of the simulations compared to traditional Central Processing Units (CPUs) by a factor of 150 on average. The convergence of the radial distribution function as a function of the so-called path integral beads for the three systems is observed. It illustrates that lighter molecules require more beads to properly account for quantum behaviour and that the quantum behaviour itself is more pronounced in lighter molecules at low temperature. Future challenges will be briefly discussed.

46 11:00 Saturday BSB-115

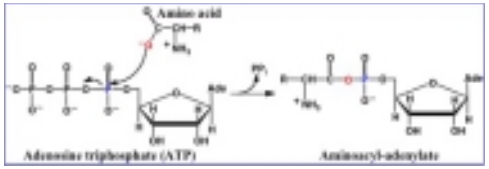
Conformational Clustering of Peptide Met-enkephalin Employing a Self-Organizing Map With Toroidal Boundaries

C. Gienow <*cg07od@brocku.ca*> and **H. Gordon** <*hgordon@brocku.ca*>, Department of Chemistry, Brock University, St. Catharines, ON, L2S 3A1.

Biological macromolecules can assume many conformations which can be difficult to classify into groups because they are described by high dimensional data (e.g. protein backbone dihedral angles). Mathematical clustering techniques are often employed; however the results are often ambiguous. It is known that Self-Organizing Map (SOM) clustering of molecular conformations has an "edge" effect, i.e. an accumulation of data along the boundaries of the map. In this study, the effect of implementing toroidal boundaries on the clustering produced by SOM was evaluated. Ensembles of conformations of the model system Met-enkephalin were generated under unsolvated and explicit solvent conditions using Nano-scale Molecular Dynamics (NAMD) and clustered to evaluate the effects of the modification to the SOM program.

47 11:20 Saturday BSB-115

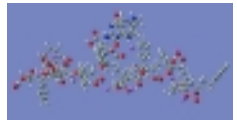
Discrimination of Cysteine from Serine: A QM/MM Study on the Activation step of Cysteinyl-tRNA Synthetase. **E. Kazim** <*kazime@uwindsor.ca*>, **G. B. Fortowsky** <*fortows@uwindsor.ca*> and **J. W. Gauld** <*gauld@uwindsor.ca*>, University of Windsor, 401 Sunset Avenue, Windsor, ON N9B 3P4.



Aminoacyl-tRNA synthetases (AARSs) are enzymes that play an important role in tRNA aminoacylation in protein biosynthesis, a process essential to the survival of all living organisms. More specifically, AARSs catalyze the attachment of amino acids to their corresponding tRNA molecules in the translational step of protein biosynthesis. Cysteinyl-tRNA synthetase (CysRS) catalyzes the attachment of cysteine to its cognate $tRNA^{Cys}$. CysRS is one of only three (3) known AARSs whose active site contains a metal ion. Furthermore, unlike many AARSs it requires no external editing of the final product for accuracy. The first-half aminoacylation reaction for AARSs has not been studied computationally. In this study, a quantum mechanical/molecular mechanical (QM/MM) approach was taken to elucidate the mechanism of the first-half aminoacylation reaction for CysRS. In addition, possible sources of how CysRS discriminates against serine were examined. The investigation revealed a concerted mechanism for the first-half reaction, containing a penta-coordinated phosphorous transition state. Also, a high energy barrier was observed when serine was substituted in the active site. The details of these key findings will be presented.

48 11:40 Saturday BSB-115

Molecular modelling of folate-conjugated PSMA nanotubes for tumor-targeted drug delivery **M.R. McTaggart** <*sm0997@rmc.ca*> and **C. Malardier-Jugroot**, Dept of Chem and Chem Eng, Royal Military College of Canada, Kingston, ON, K7K 7B4.



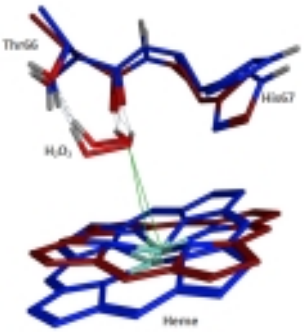
Poly(styrene-alt-maleic anhydride), PSMA, is an amphiphilic alternating copolymer that self-assembles into nanotubes in aqueous, physiological-pH environments. Folate-conjugated PSMA nanotubes could potentially transport highly toxic and hydrophobic chemotherapy agents safely through the body and selectively release their payload inside target cells by exploiting leaky tumor vasculature, folate receptor mediated endocytosis, and the pH dependence of PSMA nanostructure. Since nanotube formation and pH sensitivity are associated with oligomer linearity, functionalized PSMA moieties that retain a linear conformation are likely to retain these desirable characteristics for drug delivery.

Ab initio methods were used to model folate-conjugated PSMA geometry at the DFT-B3LYP/6-31G level of theory. Four candidate molecules were modeled by bonding diamino-poly(ethylene glycol) and 2,4-diaminobutyric acid folate derivatives to the two central carboxyl groups of a PSMA trimer. Optimized models show a linear polymer backbone at pH 7 that becomes bent at pH 3, as with unmodified PSMA. An expanded two layer ONIOM model of the 2,4-DABA variant reveals a difference between the two bonding sites that could impact nanotube self-assembly. These encouraging findings provide a pilot for further investigation into folate-conjugated PSMA as an anticancer drug delivery platform.

49 12:00 Saturday BSB-115

Coral Allene Oxide Synthase: A Mutagenic Computational Study **P. De Luna** <*deluna@uwindsor.ca*>, **E.A.C. Bushnell** <*bushne1@uwindsor.ca*> and **J.W. Gauld** <*gauld@uwindsor.ca*>, University of Windsor.

Molecular oxygen and its derivatives are essential to biological life. Coral Allene Oxide Synthase (cAOS) catalyzes the formation of reactive allene oxides from a long chain fatty acid hydro-peroxide *8R*-HPETE. On the other hand, Catalase catalyzes the decomposition of H_2O_2 to H_2O and O_2. Interestingly, cAOS's active site differs from catalase by only one residue yet has no Catalase activity. The mutation of an active site Thr66 to a Val allows cAOS to exhibit Catalase activity coupled with a decrease in native activity.[1] In order to probe the differences between wild type (WT) and mutant active sites, molecular dynamics (MD) was employed to distinguish the binding interactions of WT cAOS and T66V mutated cAOS with the native substrate and H2O2. Furthermore, a QM/MM study was performed on a sizeable active site model of T66V cAOS with H2O2 in order to elucidate the mechanism of the mutant's catalase activity. Results from this study will be presented.



(1)Tosha, T.; Uchida, T.; Brash, A. R.; Kitagawa, T. *J. Bio. Chem.* **2006,***281,* 12610.

50 09:40 Saturday BSB-120

Developing a fluorescently labelled bacterial microcrystalline cellulose substrate

A Palermo and **J Moran-Mirabal**, Department of Chemistry & Chemical Biology, McMaster University; **E Cranston**, Department of Chemical Engineering, McMaster University.

Overcoming the recalcitrance of lignocellulosic materials is the limiting factor in finding a cost-effective route for converting plant biomass into fermentable sugars for biofuel production. Therefore, an improved understanding of cellulase-cellulose interactions, including binding kinetics, is essential and may potentially lead to more effective cellulase cocktails for lignocellulose conversion on the industrial scale. The focus of this work was to develop fluorescently labelled bacterial microcrystalline cellulose (BMCC) substrates which can be employed in high resolution fluorescence microscopy studies of cellulose-cellulase interactions. The high degree of crystallinity and nanoscale cross-sectional dimensions of the material make it an attractive substrate for modelling the binding, diffusive and catalytic behaviour of cellulases. Bacterial cellulose was isolated from Nata de coco, a commercially available, food-grade bacterial cellulose source, by homogenization and NaOH purification. The resultant material was hydrolyzed using sulfuric acid to produce a stable polydisperse suspension of highly crystalline bacterial cellulose microfibrils which were characterized by atomic force microscopy (AFM), transmission electron microscopy (TEM), polarized light microscopy, and conductometric titration. BMCC was labelled using 5-(4, 6-dichlorotriazinyl)-aminofluorescein (DTAF), an organic fluorophore known to directly react with the accessible hydroxyl groups of polysaccharides. Labelled BMCC were then immobilized on a substrate for single fiber imaging by fluorescence microscopy.

51 10:00 Saturday BSB-120

Spin Gymnastics: Using Specialized Radio-Frequency Pulses to Study Unreceptive Quadrupolar Nuclei **M.J. Jaroszewicz**, **K.J. Harris**, **K.E. Johnston** and **R.W. Schurko*** <*rschurko@gmail.com*>, Department of Chemistry and Biochemistry , University of Windsor, 401 Sunset Ave., Windsor, Ontario, Canada, N9B 3P4.

Many quadrupolar nuclei have low gyromagnetic ratios, low natural abundances, large quadrupole moments, and/or unfavorable relaxation characteristics, leading to their classification as *unreceptive nuclei*. Acquiring solid-state NMR (SSNMR) spectra of unreceptive nuclei is challenging due to low S/N arising from all of the aforementioned causes. Harris *et al*. recently presented a modified cross-polarization (CP) sequence that utilizes phase-modulated, frequency-swept, adiabatic inversion pulses in lieu of conventional monochromatic spin-locking pulses.[1] It was demonstrated that using a *Wideband Uniform Rate Smooth Truncation* (WURST) pulse for x-channel spin-locking affords their broad and uniformly large frequency profiles to the transfer of polarization. This new pulse sequence, *BRoadband Adiabatic INversion CP* (BRAIN-CP), is capable of uniformly exciting broad frequency bandwidths using low power radio-frequency fields, and can be used in conjunction with broadband refocusing WURST pulses in a CPMG train. Under favourable relaxation conditions (i.e., short $T_1(^1H)$ values), S/N increases of one to two orders of magnitude are possible, along with greatly reduced experimental times. To date, BRAIN-CP has been successfully utilized for acquiring NMR spectra of transition metal spin-1/2 nuclei. We extend this work for the study of important unreceptive quadrupolar nuclei such as ^{39}K (I = 3/2), ^{25}Mg (I = 5/2), $^{47,49}Ti$ (I = 5/2, 7/2), ^{93}Nb (I = 9/2), and ^{139}La (I = 7/2), and demonstrate that BRAIN-CP can be used to acquire high quality spectra of a variety of different materials.

1. Harris *et al*. *Magn. Reson.* **2012**, *224*, 38.

52 10:20 Saturday BSB-120

Combinatorial Colourimetric Sensing: Multidimensional Differentiation of Organic Liquids **A.S. Chan** <*aschan@uwaterloo.ca*>, **B.A. Nerger**, **M.H. Kinney** and **K.P. Raymond**, Co-op Program, University of Waterloo, Waterloo, ON; **I.B. Burgess**, **N. Koay** and **J. Aizenberg**, Wyss Institute for Biologically Inspired Engineering, Harvard University, Cambridge, MA, 02138.

Chemically patterned inverse opal photonic crystals have shown great potential as colourimetric indicators. They differentiate organic liquids based on surface tension with a high degree of selectivity. The chemical non-specificity that derives from surface tension being a universal property of liquids restricts the applications of this technology as a chemical sensor. We present here a colourimetric sensory array, which exploits the wetting, drying, and liquid-liquid displacement in inverse opals to differentiate organic liquids. With the use of combinatorial approaches, this redundant yet high dimensional array successfully distinguishes between polar and aliphatic compounds. It also demonstrates remarkable prediction accuracy given a known set of organic liquids (99.99% accuracy). While this sensing platform is currently only suitable for identifying volatile organic liquids, we foresee a wide range of applications including encryption and identification of common solvents used within the lab.

53 11:00 Saturday BSB-120

Dynamic Wetting and Colour in Photoresponsive Inverse Opal Films **B.A. Nerger**, University of Waterloo, Waterloo, ON, N2L 3G1; **I.B. Burgess**, **N. Koay** and **J. Aizenberg**, Wyss Institute for Biologically Inspired Engineering, Harvard University, Cambridge, MA, 02138; **T.A. Singleton**, **A. Goulet-Hanssens** and **C.J. Barrett**, Department of Chemistry, McGill University, Montreal, QC, H3A 0G4.

Inverse-opal films (IOFs), containing a highly ordered interconnected array of spherical air pores, are well known to display brilliant iridescent colour due to coherent scattering. It has recently been shown that this highly symmetric pore structure also results in a sharply defined wetting threshold, with the transition from a completely non-wetted to a completely wetted lattice occurring over a remarkably narrow range of liquid properties. The wetting threshold can be tailored to respond to specific liquids by modifying the surface chemistry. Moreover, by patterning the surface chemistry in three dimensions using silanization and plasma oxidation, the wetting and subsequent disappearance of the IOFs iridescent colour can be manipulated to produce liquid specific patterns. Here we present the incorporation of a surface functionality that displays stimuli-responsive wetting properties, allowing the wetting state of an IOF to be dynamically controlled. We functionalized IOFs with a polyelectrolyte monolayer containing an azobenzene chromophore. Photobleaching of the chromophore was associated with increased hydrophilicity in the IOFs. By varying light exposure, the extent to which the dye was bleached and the corresponding wetting threshold of the IOF could be manipulated to a desired value. Control of wetting could also be done in situ by exposing the IOF to light while submerged in liquid, allowing dynamic control of pore infiltration.

54 11:20 Saturday BSB-120

Oxide Nanoparticles for Functional Applications **A. McEneny** <*mcen2300@mylaurier.ca*>, **N. Cathcart** <*cath9170@mylaurier.ca*> and **V. Kitaev** <*vkitaev@wlu.ca*>, Wilfrid Laurier University, 75 University Avenue West, Waterloo, Ontario, N2L 3C5.

Ruthenium, iridium and manganese dioxide nanoparticles are known to catalyze the oxidative half-reaction of water splitting. These nanoparticles behave as semiconductors whose electrons can be excited and participate in redox reactions at the semiconductor-liquid interface. However, most existing methods are hazardous to the environment, inefficient or commercially unappealing. We have prepared various ruthenium, iridium, manganese and mixed nanoparticles and investigated their photoelectrochemical activity. The general strategy for nanoparticle preparation involves using redox reactions to oxidize or reduce the metal precursor to the desired +4 oxidation state. Several systems were found to exhibit significant activity, and the best ruthenium and best manganese preparations were explored further to determine how various aspects of their preparation (volume of sample, degree of concentration, heating temperature) affects their performance. Both preparations employ water as a solvent, use environmentally benign reagents and require minimal deviation from standard conditions, increasing their commercial practicality.

55 11:40 Saturday BSB-120

Pressure-induced transformations of s-triazine and cyanuric triazide (CTA) probed by vibrational spectroscopy **E Till** <*etill@uwo.ca*>, **L Zhou** and **Y Song** <*yang.song@uwo.ca*>, Western University.

High pressure can be an effective tool in reducing the available volume and greatly increasing the electronic density so as to change the structures and properties of materials drastically. Recent discovery of diamond-like nitrogen is considered as a high energetic material because nitrogen exhibits a uniquely large difference in energy between the single bond and the triple bond. Therefore, it is of great interest to synthesize polynitrogen from other nitrogen-rich precursors by high pressures. Due to its high nitrogen content cyanuric triazide (CTA) is a promising high energetic material. S-triazine is a simpler molecule than CTA, but structurally similar, so it was hoped that it could be used as a model for preliminary understanding of the behaviour of CTA under high pressure. In this study, both CTA and s-triazine were investigated in situ under high pressure using vibrational spectroscopy. S-triazine was found to undergo an irreversible phase transition after decompression and CTA underwent an interesting phase transformation, which was indicated by a colour change as well as a difference in the Raman spectra. The behaviour of these materials provides essential information towards how nitrogen-rich compounds act under high pressure and contributes to the further understanding and developments of energetic materials.

56 12:00 Saturday BSB-120

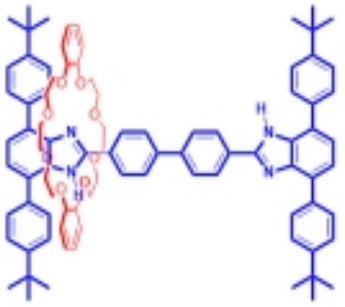
Developing Modern Undergraduate Laboratories: The Design of Light-Harvesting Dyes **B Koivisto** <*byran.koivisto@ryerson.ca*>, **B Hussein** <*burhan.hussein@ryerson.ca*>, **B Fischer** <*benjamin.fischer@ryerson.ca*>, **T Pham** <*tnpham@ryerson.ca*> and **A Sammuelsson** <*craig.sammuelsson@ryerson.ca*>, Ryerson University, 350 Victoria St, Toronto ON.

In a world where energy demand is growing, next-generation photovoltaic technologies are becoming increasely important. The dye sensitized solar cell (DSSC) is an attractive alternative where the dye is the powerhouse of the cell. Using a myriad of synthetic techniques including mircowave syntheses, cyclizations, and cross-couplings, this paper reports the development of a new senior undergraduate synthetic laboratory. These modern experiments will be dedicated to the development of dyes focusing on synthesis and physicochemical characterization (UV-Vis, electrochemical properties, theoretical calculations, etc.) of novel materials.

57 09:40 Saturday BSB-119

Benzimidazolium Based Molecular Shuttles **P Yu** <*yu119@uwindsor.ca*>, **K Zhu** <*kzhu@uwindsor.ca*> and **S.J. Loeb** <*loeb@uwindsor.ca*>, University of Windsor, Department of Chemistry & Biochemistry, Essex Hall , 401 Sunset Avenue, Windsor, ON, N9B 3P4.

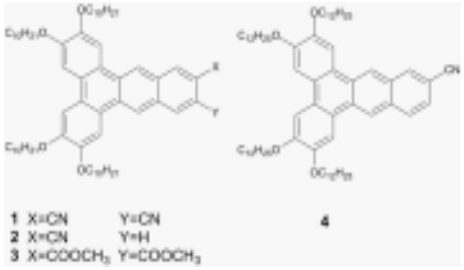
We are interested in designing ligands formed from molecular interlocked molecules (MIMs) in particular rotaxanes, and their use in the construction of metal organic frameworks (MOFs). Rotaxanes have unique properties that allow shuttling which can be controlled in response to external chemical, photochemical and electrochemical stimuli. Many [2] rotaxane molecular shuttles are large and their size is not of concern in solution. However, it is of interest to prepare compact, rigid molecular shuttles with efficient shuttling capabilities that can be incorporated into materials and devices. The synthesis and characterization of rigid, H-shaped molecular shuttles will be discussed and the shuttling rates through the control of acid-base chemistry will be presented.



58 10:00 Saturday BSB-119

Synthesis and Characterization of New Liquid Crystalline Dibenzanthracenes **A. Schneider** <*schn4170@mylaurier.ca*> and **K. Maly** <*kmaly@wlu.ca*>, Department of Chemistry, Wilfrid Laurier University, 75 University Avenue West, Waterloo Ontario N2L 3C5, Canada.

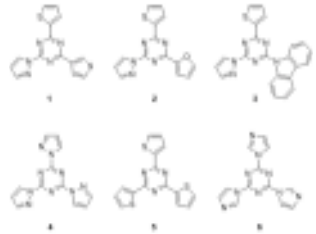
Polycyclic aromatic hydrocarbons with flexible side chains can sometimes display liquid crystallinity. In discotic liquid crystals the mesogens stack in a columnar phase which is stabilized by π-orbital overlap between adjacent aromatic cores. Varying side chains can affect the liquid crystal temperature range; however the relationship between structure and properties is not well understood. Here we will report the synthesis and characterization of a series of novel dibenz[a,c]anthracenes (**2**-**4**). Polarized optical microscopy and differential scanning calorimetry showed that compound **2** displayed a monotropic liquid crystal phase. In comparison to the previously synthesized compound **1**, compound **2** had a lower melting and clearing point in addition to a narrower liquid crystal temperature range than **1**. This comparison suggests that the presence of electron withdrawing substituents on the core stabilizes the liquid crystal phase.



59 10:20 Saturday BSB-119

Synthesis and Characterization Side-Chain Free Columnar Discotic Liquid Crystals **H. Taing** <*taingh@uwindsor.ca*> and **S.H. Eichhorn** <*eichhorn@uwindsor.ca*>, University of Windsor, Windsor, ON, N9B 3P4.

All organic semiconductors based on discotic liquid crystals contain flexible side-chains that generate an insulating layer around the conductive columnar stacks (molecular wires). This insulating layer is a disadvantage in device fabrication because it restricts charge carriers to one-dimensional transport along the columns and therefore requires perfect alignment and defect-free columnar mesophases. In addition, side-chains often complicate the purification and surface alignment of these materials. It is our objective to develop the first organic semiconductors based on side-chain free columnar discotic liquid crystals. The approach presented here intends to lower the melting point and induce columnar mesophases by an increase in conformational flexibility and minimization of the symmetry of the discotic molecule. We chose cyanuric chloride as our central core that is sequentially substituted by pyrazole, 2-thiophene, and either 3-thiophene (1), 2-furan (2), or carbazole (3). The 1,3,5-triazine reference compounds that are symmetrically substituted with three pyrazole (4), thiophene (5), or imidazole (6) units were also prepared for comparison of their melting temperatures, electronic absorption, and molecular orbital energies.

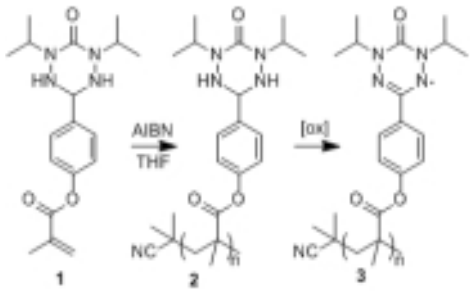


60 11:00 Saturday BSB-119

Synthesis of 6-oxotetrazane Polymers as Precursors for 6-Oxoverdazyl Radical Polymers **C. S. Harrison** <*charri73@uwo.ca*> and **J. B. Gilroy*** <*joe.gilroy@uwo.ca*>, Department of Chemistry and Center for Advanced Materials and Biomaterials Research, , Department of Chemistry, , University of Western Ontario, London, ON, Canada, N6A 5B7.

Radicals are not generally considered to be stable species, in many cases they are transient species that appear in solution and disappear rapidly, reacting with very low activation barriers.[1] However, stable, even isolable, radicals do exist and are becoming increasingly more prevalent in chemistry.[1] Stable radicals have shown utility in charge storage applications, and stable radical polymers have been developed as flexible, lightweight batteries.[2] During this presentation, the synthesis and free radical polymerization of tetrazane **1** to yield polymer **2**, a potential precursor to verdazyl radical polymer **3**, will be discussed.

1.Hicks, R. G. *Org. Biomol. Chem.*, **2007**, *5*, 1321-1338
2.Oyaizu, K.; Nishide, *H. Adv. Mater.*, **2009**, *21*, 2339-2344



61 11:20 Saturday BSB-119

Synthesis of a Series of Novel Conjugated Polymers with Tunable Electronics via Strain-Promoted Azide-Alkyne Cycloaddition Reactions. **V Kardelis** <*kardelv@mcmaster.ca*> and **A Adronov** <*adronov@mcmaster.ca*>, McMaster Universitry, 1280 Main Street West, Hamilton, Ontario , L8S 4L8.

Conjugated polymers are an interesting class of macromolecules with potential uses in the separation of carbon nanotubes. Carbon nanotubes have a wide variety of potential applications, but for their value to be realized, a method for their separation is needed. Conjugated polymers are able to interact selectively with carbon nanotubes of different band-gaps or diameter.
To further explore this phenomenon, we have synthesized a series of conjugated polymers with the unique ability to tune their electronic properties via Strain-Promoted Azide-Alkyne Cycloaddition reactions. In an eight step synthesis, dibenzosuberone was converted to a dibrominated, conjugated cyclooctyne pro-monomer, which was reacted with a series of aryl azides to produce our target monomers. Polymerization via Suzuki-Miyaura polycondensation with a diboronic ester fluorene co-monomer led to a series of homologous polymers. This talk outlines the synthesis and characterization of these polymers.

62 11:40 Saturday BSB-119

Photodegradable Polymer Vesicles **J.T. McIntosh** <*jmcint23@uwo.ca*>, **E. Gillies** and **A. Nazemi**, Western University.

Previous research has demonstrated the synthesis of block copolymers with photodegradable units along the length of the hydrophobic block and subsequent formation of micelles. We have studied and demonstrated the synthesis of an amphiphilic block copolymer with o-nitrobenzyl photosensitive moieties along the entire length of the hydrophobic block with the ability to form polymer vesicles, well-known as polymersomes. Using alkyne-azide click polymerization, an ABA-triblock copolymer was synthesized and was shown to undergo self-assembly under particular conditions to form polymersomes. The block copolymer contained a hydrophilic poly(ethylene glycol) chain bonded to a hydrophobic block of repeating o-nitrobenzyl photodegradable units. The formed polymersomes contained a hydrophobic inner compartment with the capacity for rapid disintegration and burst release of encapsulated compounds via photocleavage of the o-nitrobenzyl ester groups. These smart materials can potentially find applications in stimulus triggered controlled release of drug molecules.

63 12:00 Saturday BSB-119

Dissecting Colloidal Stabilization Factors in Crowded Polymer Solutions by Forming Self-Assembled Monolayers on Gold Nanoparticles **N. Lang** <*nj2lang@uwaterloo.ca*>, **B. Liu** <*b55liu@uwaterloo.ca*>, **X. Zhang** <*x36zhang@sciborg.uwaterloo.ca*> and **J. Liu** <*liujw@uwaterloo.ca*>, Liu Lab , Univeristy of Waterloo, 200 University Ave. W, Waterloo, Ontario, N2L 3G1.

An ideal colloidal system should be highly stable in a diverse range of buffer conditions while still retaining its surface accessibility. We recently reported that dispersing citrate-capped gold nanoparticles (AuNPs) in polymers such as polyethylene glycol (PEG) can achieve such a goal due to contributions from depletion stabilization. Since AuNPs can weakly adsorb PEG to exert steric stabilization and the remaining citrate can impart charge stabilization, the extent of the contribution of depletion stabilization is unclear. In this work, we aim to dissect the contribution of each stabilizing factor. This is achieved by coating AuNPs with a layer of thiolated compound, which inhibits the adsorption of PEG and also allows the control of surface charge. We found that depletion stabilization alone was insufficient to stabilize AuNPs at room temperature. However, when working together with other stabilization mechanisms, ultrahigh stability can be achieved. The size of both AuNPs and PEG was systematically varied and the trend was compared with theoretical calculations. Finally, we report the importance of the surface chemistry of commercial AuNPs.

64 13:40 Saturday BSB-147

Diastereoselective Indium-Mediated Approach to Chiral $C_{(3)}$-Substituted Phthalides **J.E. Curiel Tejeda** and **T. Dudding** <*tdudding@brocku.ca*>, Brock University.

Phthalides are a family of natural products found commonly throughout nature, which act as secondary metabolites in plants, bacteria and certain fungi. Several phthalides, extracted from plants, have been shown to possess broad, potent, and therapeutic biological activities in humans. Many of these compounds have been commercially developed into FDA approved drugs. The increasing interest in phthalides as pharmaceutical agents, as insecticides, and in the food industry, has led to increased interest in their synthesis. With this in mind, we have developed an indium-mediated approach to chiral $C_{(3)}$-substituted phthalides. Our approach uses a bench stable, readily available indium based catalyst, and affords phthalides in one step. Current efforts are aimed towards optimization of reaction conditions. In addition to describing our indium-mediated approach to chiral $C_{(3)}$-substituted phthalides, recent advances and future direction of indium chemistry within our research group will be discussed.

65 14:00 Saturday BSB-147

Regioselective functionalization of carbohydrates via borinic acid catalysis **T. Beale** <*tbeale@chem.utoronto.ca*>, **D. Dobrovolsky** <*dennis.dobrovolsky@mail.utoronto.ca*> and **M. Taylor** <*mtaylor@chem.utoronto.ca*>, Davenport Chemical Laboratories, 80 St. George St., University of Toronto, Toronto, Ontario, M5S 3H6.

Regioselective functionalization of hydroxyl groups in sugars is an important stepping stone toward protecting group-free synthesis and the development of greener reactions for the preparation of organic and biological compounds. We have developed borinic acid catalysts for the regioselective glycosylation, alkylation, and acylation of carbohydrates. The borinic acid catalysts our group investigates serve to activate carbohydrates towards reaction with electrophiles by binding cis-diol motifs via the boron center. Our strategy has a number of advantages over traditional methods of carbohydrate functionalization: it does not require stoichiometric quantities of toxic reagents such as organotin compounds, and circumvents the additional step normally used to install the activating group.

66 14:20 Saturday BSB-147

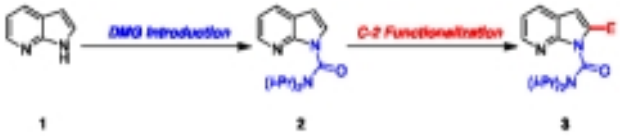
Solid-phase synthesis of peptidyl selenoesters for rapid native chemical ligation at difficult sites **A. Ghassemian**[a,b] <*ghassa@mcmaster.ca*>, [a]Department of Chemistry & Chemical Biology, McMaster University, Hamilton, ON; **P.F. Alewood** <*p.alewood@imb.uq.edu.au*> and **T. Durek** <*t.durek@imb.uq.edu.au*>, [b]Institute of Molecular Bioscience, The University of Queensland, Australia.

The chemo-selective ligation of C-terminal peptidyl thioesters with N-terminal cysteine residues allows synthetic access to medium-length peptides and proteins via native chemical ligation (NCL). However, ligation of thioesters bearing sterically hindered C-terminal amino acids shows significantly reduced ligation rates with poor yields and has traditionally been avoided. The use of peptidyl selenoesters has recently been shown to overcome the problem of slow ligation rates due to the superior leaving group ability of selenolates, thus allowing facile ligation at difficult sites. We have developed two highly optimized protocols for the synthesis of selenol-functionalized resins for solid-phase synthesis of peptidyl selenoesters for use in NCL reactions. Additionally, we characterized the hydrolytic susceptibility of peptidyl selenoesters in ligation buffers at various pH to determine stability and optimal ligation conditions. This novel methodology is a leap forward in solid-phase peptide synthesis (SPPS) and NCL techonology and serves to enhance synthetic access to peptides and small proteins by facilitating rapid NCL at difficult sites.

67 14:40 Saturday BSB-147

Regioselective Functionalization of 7-azaindole and Isomeric Derivatives <u>**M. Kaye**</u> <*8mkk2@queensu.ca*>, **M. Dalziel** <*michael.dalziel@chem.queensu.ca*>, **M. Kitching** <*kitching.matt@gmail.com*>, **C. Schneider** <*cedric.schneider@nsarouen.fr*> and **V. Snieckus** <*snieckus@chem.queensu.ca*>, Queen's University.

The 7-azaindole scaffold (1) has attracted wide interest from synthetic communities due to its presence in natural products and a variety of pharmaceutical entities. Although various methodologies have been developed for the synthesis of 7-azaindoles, the use of directed ortho metalation (DoM) using several directed metalation groups (DMGs) has enjoyed some success. While effective, some DoM methods have encountered limitations. Thus, many DMGs are limited by their ability for positional functionalization and may be resilient to subsequent derivitization. As such, application of a DMG migration, previously accomplished in the analogous benzimidazole system by Snieckus et al, [unpublished] was envisaged to be highly advantageous. The regioselective functionalization of C-2 in the 7-azaindole scaffold using the diisopropyl carbamoyl DMG, (2) (3) will be described. Further, the extension of this DoM strategy for the synthesis of substituted isomeric azaindole derivatives and heterocyclics will be described.



68 15:20 Saturday BSB-147

Towards the Total Synthesis of (±)-Paralycolin A <u>**C.-H. F. Lee**</u>, **K. G. Guimarães**, **T. E. Hurst**, **M. O. Kitching**, **A. J. M. da Silva** and **V. Snieckus**, Queen's University.

Efforts towards the total synthesis of the polycyclic natural product Paralycolin A, first isolated from the roots of *Clusia Paralycola*, will be presented. The key features of the synthesis include: a) the preparation of starting materials via Directed *ortho* Metalation (DoM) which provides the required unique substitution pattern, b) the power combination of this methodology with Heck and Suzuki-Miyaura cross-coupling tactics to synthesize sterically congested biaryls, and c) the synthetic utility of the Directed *remote* Metalation (D*re*M) to afford the requisite phenanthrol. In addition, the methodology developed to effect both the Birch reduction of the phenanthrene core and the chromene formation by a DoM strategy will be presented.

69 15:40 Saturday BSB-147

Towards the Total Synthesis of Isoprekinamycin and the Related Fluostatin Natural Products <u>**C. A. Ziebenhaus**</u> <*0cz2@queensu.ca*>, **M. O. Kitching**, **P. Jignesh** and **V. Snieckus** <*victor.snieckus@chem.queensu.ca*>, Queens University.

Efforts towards the total synthesis of Isoprekinamycin (IPK) as well as Prefluostatin, natural products obtained from Streptomyces murayamaensis and Streptomycete strain AdM21 respectively, exhibiting antibacterial and antitumor activity, will be discussed. These compounds present unique challenges due to their compact structures with problematic substitution patterns. The approach employs strategic directed metalation reactions and has the potential to be the shortest route to both IPK and Prefluostatin to date. Furthermore, progress towards the synthesis of related bioactive fluostatin family of natural products will be presented.

70 16:00 Saturday BSB-147

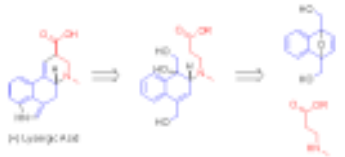
Synthesis of aza-analogues of narciclasine <u>**P. Rodriguez**</u>, **S. Vshyvenko** and **T. Hudlicky** <*thudlicky@brocku.ca*>, Brock University, 500 Glenridge Ave. , St. Catharines, ON, L2S3A1.

Narciclasine is the most potent *Amaryllidaceae* plant metabolite examined against the NIH cancer cell line panel. Despite the promising anticancer activity, the delays in human clinical trials are due to the unknown mechanism of action, and low bioavailability. Our goal is to synthesize heterocyclic analogues of narciclasine and subject them to structure-activity relationship (SAR) studies. This will determine, whether these analogues possess comparable or improved anticancer activity and/or bioavailability than the naturally occurring compound. Our approach to the synthesis of the aromatic A-ring of the heterocyclic analogues will be discussed along with future directions towards the completion of synthesis.

71 16:20 Saturday BSB-147

Towards the Total Synthesis of Lysergic Acid via Rh-Catalyzed Asymmetric Ring Opening **J. Tsoung** <*jtsoung@chem.utoronto.ca*>, <u>**E. K. J. Lui**</u> <*erica.lui@mail.utoronto.ca*> and **M. Lautens** <*mlautens@chem.utoronto.ca*>, Chemistry Department, University of Toronto, Toronto, ON, M5S3H6; **A. Boyer** <*Alistair.Boyer@glasgow.ac.uk*>, School of Chemistry, University of Glasgow, Scotland.

Lysergic acid belongs to the ergoline alkaloids, whose members have displayed important biological activities. Notably, they have been used in clinical treatments for Parkinson's disease and depression. There have been thirteen total syntheses of this molecule, and only four of them were enantioselective variants; however, most syntheses utilized Uhle's ketone or a pre-constructed indole motif. We have designed a novel strategy towards this complex alkaloid involving the Rh(I)-catalyzed asymmetric ring opening (ARO) of oxabicyclic alkenes developed in our group. This desymmetrization reaction provides the benzo-fused skeleton present in the target molecule with the correct stereochemistry, from which we can easily access the indole motif.



72 13:40 Saturday BSB-117

Carbonyl Sulfide Decomposition on Cationic Rhodium Clusters <u>**W.C.T. Chow**</u> <*wctchow@uwaterloo.ca*>, **M.J. Lecours** <*mjlecour@uwaterloo.ca*> and **W.S. Hopkins** <*shopkins@uwaterloo.ca*>, Department of Chemistry, University of Waterloo, 200 University Avenue West, Waterloo, Ontario, N2L 3G1.

The dramatic size-dependent variation of physico-chemical properties for transition metal (TM) clusters has attracted a great deal of interest in recent years. Determining if TM_n clusters may be viewed as model cases for bulk processes (*e.g.* heterogenous catalysis), or if they exhibit unique properties quite dissimilar from the bulk or their constituent atoms, is a major theme in cluster research. Rhodium, in particular, has received quite a bit of attention owing to its industrially important catalytic properties. For example, Rh is used as a reduction catalyst in the automobile three-way converter.

Sulfur is known to poison bulk catalysts. Whether or not the same is true of nanostructured materials is still an open question. In this computational study, the decomposition of carbonyl sulfide (OCS) on Rh_n^+ (n = 3-12) is examined as a model system of the three-way converter. The basin-hopping search strategy is used to identify low-energy minima on cluster potential energy surfaces, thereby generating an unbiased test set for high-level density functional theory electronic structure calculations. Preliminary results show that OCS favours a linear S-bound binding motif. As the Rh_n^+ cluster core increases in size, rearrangement of the surface-bound OCS occurs and activation of the C-S bond leads to decomposition and loss of carbon monoxide.

73 14:00 Saturday BSB-117

Towards the Syntheses of Mercury(IV) Compounds **J.R. DeBackere**, **H.P.A. Mercier** and **G.J. Schrobilgen**, McMaster University.

Among the group 12 elements, mercury appears to be most suited for the synthesis of Hg(IV) species. A recent matrix-isolation study has provided evidence for $Hg^{IV}F_4$, which decomposed to HgF_2 and F_2 upon warming.[1] Quantum-chemical calculations (QCC) indicate that derivatives of the highly electronegative $OChF_5$ (Ch = Se, Te) groups could provide avenues to the bulk syntheses of Hg(IV) compounds, e.g., $Hg(OChF_5)_4$.[2] In the present work the synthetic precursor, $Hg(OTeF_5)_2$, has been synthesized in high purity and high yield and structurally characterized, along with its coordination complexes, cis, trans-$(F_5TeO)_2Hg(NCCH_3)_4$ and $2[(F_5TeO)_2Hg]3XeF_2$ (Figure 1). The latter compounds were characterized by low-temperature single-crystal X-ray diffraction, Raman spectroscopy (RAS) and QCC. It has also been shown by RAS that a KrF_2 coordination complex with $Hg(OTeF_5)_2$ may be formed.

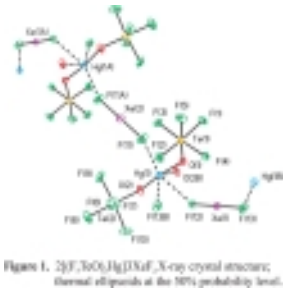


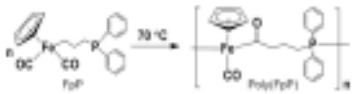
Figure 1. $2[(F_5TeO)_2Hg]3XeF_2$ X-ray crystal structure; thermal ellipsoids at the 50% probability level.

1. X. Wang, L.S. Andrews, S. Riedel, M. Kaupp, *Angew. Chem. Int. Ed.***2007**, *46*, 83718375.
2. S. Riedel, M. Straka, M. Kaupp, *Chem. Eur. J.***2005**, *11*, 27432755.

74 14:20 Saturday BSB-117

Migration Insertion Polymerization: A New Concept for Main Chain Metal Containing Polymers. **X. Wang** <*xiaosong.wang@uwaterloo.ca*>, Department of Chemistry and Waterloo Institute of Nanotechnology, , University of Waterloo,, 200 University Avenue, , Waterloo, ON, N2L 3G1.

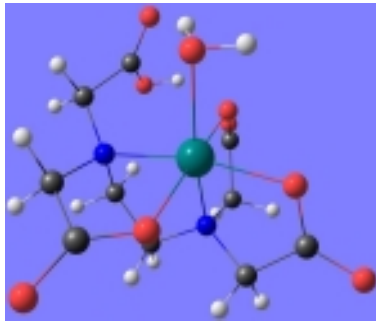
The progress of synthetic chemistry for metal containing polymers (MCPs) has led to the creation of many new MCPs with desirable magnetic, conductive, optical and catalytical properties. In order to access new types of MCPs for material applications, we developed a new concept for synthesizing MCPs using organometallic migration insertion reactions (MIR) along with A-B type difunctional monomers. This new concept is termed migration insertion polymerization (MIP). As a proof of concept, Cyclopentadienyl(dicarbonyl)(diphenylphosphinopropyl) iron (FpP) is synthesized as an A-B type difunctional monomer with a Fp group capable of MIR at one end, and a phosphine group acting as an incoming neutral ligand at the other end. At an elevated temperature, MIP occurs producing air stable Poly(FpP). GPC analysis have demonstrated that Poly(FpP) displays a high molecular weight with narrow molecular weight distribution (PDI = 1.08-1.33). Through NMR spectroscopy characterization, Poly(FpP) have been shown to contain asymmetric iron units connected by both phosphine coordination and Fe-acyl bonds, which is representative of a new class of polymers.



75 14:40 Saturday BSB-117

Ru(II)-EDTA complex as a water, acid and high-temperature stable deoxygenation catalyst **R Sullivan** <*rsulliva@uoguelph.ca*> and **M Schlaf** <*mschlaf@uoguelph.ca*>, University of Guelph.

A complex between ruthenium (II) and ethylenediaminetetraacetate has been formed in situ and investigated as an acid, water and high-temperature stable catalyst for the deoxygenation of biomass derived substrates to suitable materials for use as petrochemical feedstocks. Evaluation of catalytic activity has been performed using sorbitol and 2,5-hexandione (a model substrate for furfural type biomass products).



76 15:20 Saturday BSB-117

Synthesis and investigation of novel thermoelectric suboxides: $Gd_2Bi_{1-x}Sb_xO_2$, $Sm_2Bi_{1-x}Sb_xO_2$, $Ho_2Bi_{1-x}Te_xO_2$ **L. J. Ogilvie** <*ogilvilj@mcmaster.ca*> and **Y. Mozharivskyj** <*mozhar@mcmaster.ca*>, McMaster University.

Properties of a thermoelectric material are governed by an internal trade-off between the Seebeck coefficient and electrical conductivity, both of which depend on the carrier concentration. This internal trade-off affects the material performance as well as limits the efficiency of chemical doping. RE_2BiO_2 and RE_2SbO_2 have previously been studied; in these materials both the Seebeck coefficient and electrical conductivity increase, however without a change in the charge carrier concentration. New RE systems have been synthesized in order to probe the relationship between the local crystal structure and thermoelectric properties. $RE_2Bi_{1-x}Sb_xO_2$ was prepared for RE = Gd, Sm and electrical resistivity was measured. Electrical resistivity decreases for both Gd and Sm series when Bi is replaced by Sb. In the $Ho_2Bi_{1-x}Te_xO_2$ system, the phases of interest were prepared with relatively good purity.

77 15:40 Saturday BSB-117

Targeting Fluorinated Organic Molecules via Perfluorometallacycle Activation **N.O. Andrella**[a,b] <*nandr046@uottawa.ca*> and **R.T. Baker**[a,b] <*rbaker@uottawa.ca*>, [a]University of Ottawa, , 75 Laurier Avenue East, Ottawa, ON , K1N 6N5; [b]Centre for Catalysis Research and Innovation, 30 Marie-Curie, Ottawa, ON, K1N 6N5.

Fluorinated organic molecules have found utility in a wide range of areas, including as solvents, surfactants, refrigerants, anesthetics and as organofluorine building blocks (e.g. for pharmaceuticals). [1] However, the manufacturing processes of these compounds typically involve the use of elemental fluorine. [2] Transition metal-catalyzed routes could provide low-cost and efficient alternatives to these syntheses, but the successful implementation of these metal-mediated processes has thus far been limited. [3] In a rare example of metal perfluoroalkyl bond activation, Baker et al. demonstrated the catalytic hydrodimerization of tetrafluoroethylene. [4] With this in mind, the primary goals of this project are to explore the preparation of high oxidation state nickel metallacycles that could facilitate catalytic turnover of Ni-bound perfluoroalkyl species. [5] Results to be presented include the synthesis and characterization of several Ni^{III} species, the synthesis of nickel hexafluoropropene complexes, the synthesis of a 3-coordinate Ni^{II} species, and ongoing attempts to prepare a Ni^{IV} perfluorometallacycle.

References:

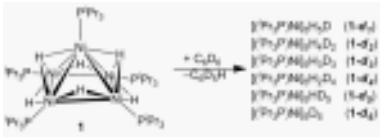
[1] Kirsch, D. P. *Modern Fluoroorganic Chemistry: Synthesis, Reactivity, Applications*, Darmstadt: WILEY-VCH, 2004. [2] Chambers, R.D. *Organofluorine Chemistry: Techniques and Synthons*, Berlin: Springer-Verlag, 1997. [3] For selected examples see: Ogoshi, S. et al. *Eur. J. Org. Chem.* **2013**, 443447; Buchwald, S. L. et al. *J. Org. Chem.* **2011**, *76*, 11741176 [4] Baker, R. T. et al. Process for the manufacture of selected halogenated hydrocarbons containing fluorine and hydrogen and compositions provided therein. US Patent No. 5,760,282, 1998. [5] Schwiebert, K.; Stryker, J. M. *J. Am. Chem. Soc.***1994**, *116*, 11570.

78 16:00 Saturday BSB-117

A Mechanistic Investigation of H/D Exchange of Unactivated C-H bonds from a Pentanuclear Nickel Cluster **M Shoshani** <*shoshanm@uwindsor,ca*> and **S.A Johnson**, University of Windsor.

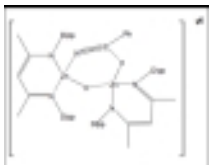
A pentanuclear nickel cluster was found to exchange deuterium into unactivated C-H bonds. C-H bonds generally have large dissociation energies which allow them to be resistant to various chemical transformations. Several mechanisms of C-H activation exist, including more common mechanisms such as oxidative addition and sigma-bond metathesis. Unactivated C-H bonds are found in common laboratory solvents such as benzene, toluene and THF. The pentanuclear nickel cluster Ni5L5H6 (L=PiPr3) was shown to activate C-D bonds from several deuterated complexes while exchanging hydrogen from the hydride in the cluster. The process resulted in the observation of several isotopologues via 31P{1H} and 1H NMR. The cluster has a strong temperature dependence to chemical shift suggesting a singlet ground state and a low lying triplet state. Studies to better understand the mechanism of C-H activation will be discussed.

Beck, R; Shoshani, M; Johnson, S.A. Angew. Chem. Int. Ed.2012, 47, 11923-11926.



79 16:20 Saturday BSB-117

Catalytic and Mechanistic Studies of Hydrosilylation Mediated by a Zinc Hydride Complex **C. Boone** and **G.I. Nikonov**, Brock University, Department of Chemistry, St. Catharines, Ontario, Canada L2S 3A1.



The monomeric zinc hydride complex DippNacNacZnH (**1**, DippNacNac = CH{(CMe)(2,6-$iPr_2C_6H_3N$)}$_2$) containing a three-coordinate zinc center was synthesized by reacting the zinc chloride precursor DippNacNacZnCl with potassium *tert*-butoxide followed by the addition of phenylsilane. Complex **1** was shown to catalyze the hydrosilylation of nitriles, ketones and aldehydes. Mechanistic studies were first carried out for the insertion of benzonitrile into the zinc-hydride bond of **1** to give the intermediate DippNacNacZn-N=C(H)(Ph). Unexpectedly, the reaction rate of insertion was found to be second-order with respect to **1**. At high concentrations of benzonitrile (8-12 eq), the reaction showed saturation behaviour allowing for kinetic measurements. The entropy of activation and enthalpy of activation were calculated to be -272 J/molK and 17.7 kJ/mol, respectively. We propose that the reaction proceeds via a six-membered transition state, involving two molecules of **1** and one molecule of benzonitrile.

Surprisingly, the DippNacNacZn-N=C(H)(Ph) complex showed no reactivity toward silane, which indicates that the hydrosilylation mechanism does not go through this intermediate. Mechanistic studies were then carried out for the hydrosilylation of benzonitrile with $(EtO)_3SiH$ catalyzed by **1**. The reaction showed saturation behaviour at high concentrations of benzonitrile. Our proposed mechanism involves coordination of silane to **1** to form an intermediate, which then reacts with benzonitrile to give the silylimine product and regenerate **1**.

80 13:40 Saturday BSB-121

Comparative study of three ruthenium (II) polypyridyl complexes in dye-sensitized solar cells **S. Abner** <*sharon28@yorku.ca*>, **S. Morin** <*smorin@yorku.ca*> and **A. Sepehrifard** <*ali.sepehri@gmail.com*>, York University.

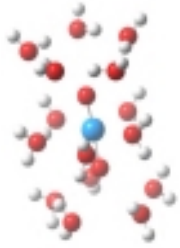
Due to the depletion of fossil fuel and global warming, the necessity of an environmentally and ecologically friendly energy source is urgent. The development of Dye-Sensitized Solar Cells (DSSC) by Michael Grätzel and Brian O'Regan in 1991 introduced an alternative method to the traditional and expensive solid-state photovoltaic techniques. The DSSC is a low cost and a simply assembled device that converts solar energy to electricity with maximum efficiency of ca. 12% conversion.

This project focuses on correlating the photo-physical properties of the dyes analyzed to their structures and to provide a benchmark for synthesis of sensitizers with improved properties. Three ruthenium (II) polypyridyl complexes, BB1, BB2, and BB3 (Figure 1), were analyzed and compared to a N3 dye in DSSCs prepared with an iodide/triiodide electrolyte. The dye's absorption spectra were measured to be in the range of 550 450 nm. The HOMO energy levels of BB1 BB3 dyes were estimated by cyclic voltammetry to be 1.15, 1.19, and 1.16 V vs. NHE, respectively. The band gaps of the dyes were estimated to be 2.26, 2.19, and 2.30 eV, respectively, by UV-VIS spectroscopy. Photocurrent-Voltage experiments were conducted to determine the efficiencies of BB1 - BB3 in the DSSCs and are as follows: 0.02%, 0.09%, and 0.03%, compared to a value of 2.61% for N3 under the same conditions. Lastly the dye's adsorption to the titanium dioxide layer was quantified by UV-Visible spectroscopy.

81 14:00 Saturday BSB-121

Microsolvation of Uranyl, UO2+

Ceramic pellets of uranium dioxide are used a fissionable fuel source in Canadian uranium deuterium (CANDU) reactor. To improve efficiency, generation IV reactors have been proposed that will employ supercritical water (SCW) as the working fluid and coolant in a closed-loop cycle. The study of uranyl (UO22+) salt properties has important implications to the design of the new SCW reactor. In particular, UO2+ solubility under high temperature water (turbine) and SCW (reactor core) conditions are of interest.



We have undertaken an extensive computational study of UO2+ aqueous microsolvation, bothin the presence and absence of counterion species which may be present in SCW reactors due to condenser leaks. A basin-hopping search of the associated potential energy surface identifies candidate UO2+X(H2O)n structures that are thermodynamically accessible. These structures are then employed as a test set for high-level density functional theory electronic structure calculations. Through building the clusters a single water molecule at a time, we effectively take snap-shots of the solvation process. Normal mode analysis shows whether these structures are stable isomeric forms or transition states for isomerisation processes. At each step, infrared and Raman spectra are predicted to serve as a guide for interpretation of results from planned future experiments.

82 14:20 Saturday BSB-121

Investigating the Adsorption of Organic Compounds in MOF MIL-53 **B. Ibrahim** <*bibrahi@uwo.ca*>, **J. Xu** <*jxu252@uwo.ca*> and **Y. Huang** <*yhuang@uwo.ca*>, Department of Chemistry, The University of Western Ontario, London, Ontario, N6A 3K7.

Metal-organic frameworks (MOFs) are a versatile class of porous materials that are being heavily studied due to the wide variety of elements used to make these materials, the ability to modify and design the pores by selecting different organic linkers, and the numerous applications of these MOFs. MIL-53 (Al), Al(OH)[O2C-C6H4-CO2], is made up of corner sharing Al octahedral connected by 1,4-benzenedicarboxylate linkers and belongs to a unique class of MOFs with flexible frameworks. The framework exhibits a breathing effect, a change in pore dimensions, caused by interactions between guest adsorbates and the framework. Through thermal gravimetric analysis (TGA), x-ray diffraction (XRD), and ^{27}Al magic-angle spinning solid-state nuclear magnetic spectroscopy (^{27}Al MAS-SS-NMR), a three-pronged approach was used to study the interactions between various organic guest compounds and the framework. TGA was used to determine the amount of adsorbate per unit cell, and to understand how strongly the adsorbates interact with the framework based on desorption temperatures. XRD was used to monitor the changes in the crystal structure induced by the interactions between the adsorbates and the framework. Finally, ^{27}Al MAS-SS-NMR was used to study the changes in the ^{27}Al local environment.

83 14:40 Saturday BSB-121

Insertion Complexes of Cyclic Organic Molecules Trapped in Metal-Halide Ion-pairs **B.S. Cochrane** <*emailbrycecochrane@gmail.com*> and **F.Y. Naumkin** <*fedor.naumkin@uoit.ca*>, Faculty of Science, University of Ontario Institure of Technology, 2000 Simcoe Street North Oshawa, Ontario, Canada L1H 7K4.

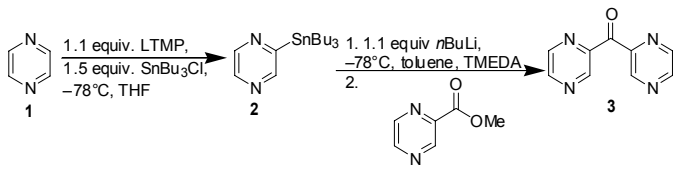
A group of novel molecule-insertion complexes MC_4H_8X (MX = alkali-halide) is introduced and studied computationally. Charge distributions for the complexes indicate that cyclobutane (C_4H_8) is essentially neutral when trapped between the two opposite ions. In such a system, cyclobutane is predicted to adopt a flat conformation of its carbon ring. Effects of electron attachment on the structure and stability are investigated for corresponding anions. Two such systems are then merged into a dimer MC_4H_8X-MC_4H_8X as a step towards a polymer chain of the ion-pair-trapped-molecule units. For the purposes of investigating further options, cubane (C_8H_8) and cyclobutadiene (C_4H_4) based counterparts are also studied. System stabilities for different dissociation channels and structure perturbations of each complex are discussed and interpreted, in particular to give insight for energy storage. Other features of interest include very large dipole moments (hence possible use for optical sensors), potential molecular-switch applications and further structural extensions to ion-pair linked 2D and 3D organic frameworks up to materials.

84 15:20 Saturday BSB-121

Synthesis of dipyrazinyl ketone by transmetalation of 2-tributylstannanyl pyrazine **K. Emberson** <*ke08tg@brocku.ca*>, **C. Metallinos*** <*cmetallinos@brocku.ca*> and **T. Stamatatos** <*tstamatatos@brocku.ca*>, Brock University.

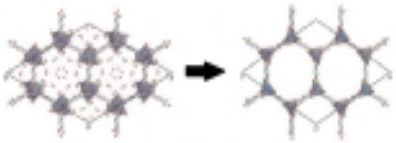
The focus of this project is to find an alternative synthesis of $(pyz)_2CO$ ligand (3), which is anticipated to be used in place of the commercially-available ligand $(py)_2CO$ in polynuclear metal cluster chemistry. An alternative two step synthesis of the ligand was established starting from pyrazine, rather than the much more expensive 2-iodipyrazine reported previously by Mak and Wang.1 It is expected that upon metal-assisted hydration of the $(pyz)_2CO$ ligand, the resulting dipyrazinediolate group will have six donors atoms (N,N,N,N,O,O) for coordination with the metal centers, compared to the four donor atoms (N,N,O,O) available for the hydrated $(py)_2CO$ ligand. It is then obvious that the $(pyz)_2C(OH)_2$ group will lead to new molecular species with larger nuclearities and much more impressive structural motifs compared with $(py)_2C(OH)_2$; the exact nuclearity of which is impossible to predict and design provided that the synthetic attempts will be based on serendipitous assembly. Investigation into its coordination chemistry are ongoing.

1.Wang, C.Q.; Mak, T.C.W. *Inorganica Chimica Acta* **2008**, *361*, 1496.



85 15:40 Saturday BSB-121

Characterization of Metal-Organic Framework using Solid-State ^{2}H NMR and X-ray Absorption Spectroscopy **R. Sinelnikov** <*rsinelni@uwo.ca*>, **J. Xu** <*jxu252@uwo.ca*>, **T.K. Sham** <*tsham@uwo.ca*> and **Y. Huang** <*yhuang@uwo.ca*>, The University of Western Ontario, London, Ontario, N6A 5B7.



Investigation of the local environment of metal-organic frameworks (MOFs) is of interest due to their potential application in gas storage, gas separation and catalysis. The isostructural series of MOFs CPO-27-M (M = Zn, Mg) has a vacant coordination site on the metal centre upon dehydration. The empty site can be occupied by guest molecules, and in particular CPO-27-Mg was shown to have exceptional CO_2 adsorption capabilities. In this study, the effects of dehydration and introduction of guest molecules on the local environment of CPO-27-M were studied. ^{2}H Solid-State NMR was used to study the motional dynamics of deuterated acetone, pyridine, benzene and water guest molecules in the framework. Additionally, X-ray Absorption Spectroscopy (XAFS) was used to probe the local environment of the metal centre in the hydrated, dehydrated and loaded with guest molecule forms.The results of the experiments have shown that the strength of interaction of the framework with the guest molecules strongly depends on the nature of the metal centre. Furthermore, dehydration and introduction of guest molecules distorted the local order of the metal. ^{2}H SSNMR and XAFS were shown to be complementary techniques that can provide comprehensive picture of the local environment of metal-organic frameworks.

86 16:00 Saturday BSB-121

Binding Manganese to Metallothionein **M. Assaf** <*massaf23@uwo.ca*> and **M. Stillman** <*martin.stillman@uwo.ca*>, The University of Western Ontario, Richmond St., London, ON.

The naturally occurring metallothionein is a low molecular weight, cysteine rich and a well-known metal binding protein. Originally discovered in the equine tissue, metallothionein can be found in humans as well. The mammalian metallothionein is composed of two domains which can readily bind divalent metals of Group 11 and 12; the alpha domain consists of 11 cysteines and produces a 4 metal-thiolate cluster whereas the beta domain contains only 9 cysteines, thereby producing a 3 metal-thiolate cluster. Manganese is the 12th most abundant element and the 3rd most abundant transition metal on earth. It is an essential trace element found in the body, where it accumulates in the mitochondria, and carries out its functions in the body through metalloenzymes like arginase, pyruvate carboxylase and superoxide dismutase. From the Periodic Table, metals surrounding manganese, like iron, technetium and cobalt have all been shown to bind to metallothionein. However, being a hard metal, it has been a challenge to predict whether or not manganese will bind to the protein. The binding of manganese to recombinant human metallothionein (rh-MT1a) in its metal free state was studied by electrospray ionization mass spectrometry (ESI-MS).

87 16:20 Saturday BSB-121

Alkali-Metal Derivatives of Highly-Charged Conjugated Anions **V. Somasundaram** <*somasv@mcmaster.ca*>, McMaster University,1280 Main St. W., Hamilton, ON L8S 4M1.

Due to its durability, storage capacity and large current delivery, the rechargeable lithium ion battery is one of the most popular devices used for energy storage. Despite many recent improvements to the design of such devices, the anode is still made of graphite, which is difficult to modify in order to enhance its properties. We are pursuing alternative anode materials based on organic structures that can take a large number of electrons reversibly. As an example, bis-iminoacenaphthenes (BIAN) can acquire a -4 charge and a macromolecular material based on such building blocks could store more electrons per unit of mass than graphite. One open question, however, is whether a high density of negative charge will degrade the acceptor ability of BIAN. In an attempt to examine this issue, we are studying how far BIAN derivatives can be reduced when they bear peripheral anionic groups.

88 13:40 Saturday BSB-136

A Novel Function of Cystathionine-ϒ-lyase: Disulfide Reductase **Y. Atwan** <*atwany@uwindsor.ca*>, **A. Faccenda** <*faccen2@uwindsor.ca*> and **B. Mutus** <*mutusb@uwindsor.ca*>, University of Windsor, Departement of Chemistry & Biochemistry, Windsor, ON.

Cystathionine-ϒ-lyase (CGL) is the enzyme predominately responsible for the production of hydrogen sulfide (H_2S) in the periphery for various physiological processes. Examination of the amino acid sequence of CGL reveals the presence of two CXXC motifs per subunit of the homotetramer; a motif common to enzymes in the Thioredoxin superfamily. This discovery led us to examine whether CGL displays disulfide reductase activity, most commonly associated with the Thioredoxin superfamily.

By utilizing Dieosin Glutathione Disulfide (Di-E-GSSG), a fluorescent probe developed in our lab, evidence was obtained indicating CGL is capable of not only of catalyzing the production of H_2S, but may also act as a disulfide reductase; which was a previously unknown function. The enzyme was found to have a K_M of 155 nM for Di-E-GSSG. Furthermore, in order to elucidate the residues mainly associated with CGL reductase activity, site directed mutagenesis was conducted. Mutations C252S and C307S of unique CXXC motifs were obtained and the purified enzymes were examined to have a K_M of 76 nM and 90 nM for the respective mutations. These results indicate a possible presence of a unique motif responsible for the CGL reductase activity.

89 14:00 Saturday BSB-136

Investigation of the effect of glutamine and its metabolites on the phosphorylation of mTORC1 targets **G Desmarais** <*gx_desmarais@laurentian.ca*>, **A Abusneina** and **E Gauthier** <*egauthier@laurentian.ca*>, Laurentian University.

Sp2/0-Ag14 murine hybridoma cells are a useful tool for the study of the phenomena of L-Glutamine (Gln) dependence in cancer, as Gln deprivation leads to rapid onset of apoptosis in these cells. Preliminary data shows that ammonia, a product of glutaminolysis, partially protects Sp2/0-Ag14 from Gln deprivation induced death. We investigated the capacity of Gln and its metabolites to induce phosphorylation of effectors of the mTORC1 pathway, a well established nutrient sensor. Through Western blotting, we demonstrate that Gln deprivation for 2hrs in Sp2/0-Ag14 causes dephosphorylation of mTORC1 targets S6k (Thr 389) and 4EBP-1 (Thr 37/46 and Ser 65). This suggests that mTORC1 could serve as a possible mechanism of detection of Gln in Sp2/0-Ag14. Interestingly, ammonia supplementation during Gln deprivation preserved phosphorylation of 4-EBP-1 at Thr 37/46. However, ammonia did not prevent dephosphorylation of 4EBP-1 Ser 65 or S6k Thr 389. Our results suggest that ammonia, a product of glutaminolysis, modulates mTORC1. Whether this is part of the cellular mechanism linking Gln to cell survival remains to be determined (funded by NSERC).

90 14:20 Saturday BSB-136

Functional consequences of NOx-modification on cystathionine-γ-lyase. **H Ali Khan** <*alikha@uwindsor.ca*>, **A Faccenda** <*faccen2@uwindsor.ca*>, **J Wang** and **B Mutus** <*mutusb@uwindsor.ca*>, University of Windsor, Windsor, ON, N9B 3P4.

When hydrogen sulfide (H_2S) was determined to be a gasotransmitter, there was an exponential increase in interest in its biological role. From these studies it has been determined that cystathionine-γ-lyase is the major enzyme that produces H_2S in humans. Research has indicated that H_2S has a role in vasodilation, inflammatory response, as well as a possible role in mediating hypoxic effects. Interestingly another gasotransmitter, nitric oxide (NO), has many similar roles as H_2S in humans. This indicates that there is a possible interaction between the two gasotransmitters. This study focuses on NO's affect on H_2S production from cystathionine-γ-lyase under normoxic and hypoxic conditions *in vitro*. A novel technique for H_2S detection, developed in our lab, was used in this experiment, which utilizes polydimethylsiloxane permeability-based wells to select for H_2S. The H_2S is then quantified by its reaction with DTNB, which can be detected in real time. The results from this study show that NO has minimal effect on enzyme-substrate binding affinity with the substrate cysteine, under normoxic conditions. The Michaelis constant (K_M) increased from 4.7mM without a nitric oxide donor to 9.9mM with a nitric oxide donor under normoxia. Under hypoxic conditions however, NO was shown to have a significant effect on enzyme-substrate binding affinity with cysteine as the substrate, evidenced by an increase in K_M from 13mM with no nitric oxide donor, to 44mM with a nitric oxide donor. The findings of this study indicate a possible role of NO as a regulator of H_2S production by cystathionine-γ-lyase. Further studies include performing *in vivo* assessments to validate these findings.

91 14:40 Saturday BSB-136

DAHP Synthase: Oxime Inhibition and Dynamic Studies on an Antibiotic Target **E.J. Curiel Tejeda** and **P.J. Berti**, McMaster University.

The discovery and development of antibiotics was the biggest medical advance of the 20th century, but this is all being threatened by the accelerating spread of antibiotic resistance throughout the world. Our group focuses on understanding and characterizing enzymes' transition states (TSs) in order to develop powerful new inhibitors. 3-Deoxy-D-arabino-heptulosonate 7-phosphate synthase (DAHPS) is an enzyme of the α-carboxyketose synthase superfamily that is responsible for the first committed step of aromatic amino acid biosynthesis in bacteria, and it has become an attractive target for drug development. We identified that oxime inhibitors are potent inhibitors, with Ki* = 3 nM for the DAHPS(Phe) isozyme, but its true mechanism of binding is still unknown due to the unknown TS of the enzyme itself. Hydrogen-deuterium exchange dynamic studies on the Phe-isozyme demonstrated that there is a significant change in protein dynamics upon oxime binding relative to the natural substrates. To further expand on this study, we are kinetically characterizing the DAHPS(Tyr) with the oxime inhibitor and further perform dynamic studies at the residue level. We will use 19F-trp NMR and 15N-Trp TROSY NMR to understand the effects of substrate and inhibitor binding on enzyme dynamics and improve our understanding of TSs and catalysis mechanism.

92 15:20 Saturday BSB-136

Identifying novel natural product inhibitors of the 1-deoxy-D-xylulose 5-phosphate pathway. T.E. Chung <*chungte@mcmaster.ca*>, Department of Chemistry and Chemical Biology, McMaster University, Hamilton, Ontario, Canada L8N 3Z5; **T. Czarny** and **E.D. Brown**, M. G. DeGroote Institute for Infectious Disease Research and Department of Biochemistry and Biomedical Sciences, McMaster University, Hamilton, Ontario, Canada L8N 3Z5.

Isoprenoids are essential in all living organisms and are biosynthesized from two universal precursors: isopentenyl pyrophosphate (IPP) and dimethylallyl pyrophosphate (DMAPP). In nature, two unrelated pathways synthesize these precursors: the mevalonate (MEV) pathway, used by eukaryotes and archaebacteria, and the 1-deoxy-D-xylulose 5-phosphate (DOXP) pathway, utilised by most eubacteria (an exception being Staphylococcus aureus). Since the DOXP pathway is essential in many bacteria and absent in humans, it presents an excellent target for novel antibiotics.

To identify novel DOXP pathway inhibitors, we performed a high-throughput screen on bacterial extracts from the Wright Actinomyces Collection (WAC) Natural Product Library, against two strains of Bacillus subtilis 168: a wild-type strain and a strain of B. subtilis 168 engineered to express the S. aureus MEV pathway under xylose control (EB2337). Extracts with specific activity against the DOXP pathway should inhibit the growth of wild-type B. subtilis but not EB2337 since it can continue synthesizing IPP and DMAPP via the MEV pathway. Of the 4080 extracts screened, 27 were identified to inhibit the DOXP pathway. The activity of 8 of these extracts were reproduced in a refermentation. Efforts are now underway to isolate the active compounds from these extracts.

93 15:40 Saturday BSB-136

The Impact of *Cis*-Regulatory Variation on *Drosophila melanogaster* Malic Enzyme Biochemistry K Gallagher <*km_gallagher@laurentian.ca*> and **T Merritt** <*tmerritt@laurentian.ca*>, Laurentian University, Sudbury, ON, P3E2C6.

In eukaryotes, a larger fraction of the genome is made up of regulatory elements than amino acid coding sequences. It is gene regulation that drives biological complexity and diversity, but most regulatory elements, and their exact biological functions, have yet to be identified. Almost all regulation of gene expression is due to *cis*-interactions between regulatory elements and coding regions within a locus. This study seeks to gain a greater understanding of how regulatory DNA variation can affect gene expression and drive phenotype in a wild-population. We sequenced 4kb of the 5' region of the *D. melanogaster Malic enzyme (Men)* locus from 26 individuals from a local fly population. Within this population are two structural (amino acid) alleles that have previously been shown to exhibit different enzyme biochemistry. Characterization of malic enzyme (MEN) is conducted in order to uncover any natural regulatory variation that may further explain biochemical variation. This characterization is carried out at three molecular levels: 1) the genomic level via sequencing DNA upstream of the transcription start site of *Men*, 2) the mRNA level by quantification of *Men* expression, and 3) the protein level by quantifying MEN activity via Vmax. Algoritmic analysis of divergence/convergence of the sequence data is compared to activity and gene expression levels. Four naturally derived polymorphisms were shown to significantly impact MEN activity. Further, combinations of these alleles were shown to result in potentially additive effects. The results of this study provide insight into possible regulatory regions of *Men*, and can influence further mapping of the *D. melanogaster* chromosomes.

94 16:00 Saturday BSB-136

Expression and purification of Bacterial Cellulose Synthase Protein E from *Escherichia coli* L.F. Kell <*kell2740@mylaurier.ca*>, **M. Jelokhani-Niaraki** and **J.T. Weadge**, Wilfrid Laurier University, Waterloo, Ontario.

Biofilms are composed of exopolysaccharides secreted by bacteria. These extracellular matrices confer protection against mechanical stress and host defences as well as chemical resistance to antimicrobial agents and disinfectants, such as chlorine. This leads to persistent colonization of these bacteria which has implications in food contamination and chronic infections. One of the major constituents of biofilms associated with *Escherichia* and *Salmonella* spp. is cellulose. Cellulose production, excretion and degredation is a result of the bacterial cellulose synthase system, a cluster of proteins which form complex spanning the inner membrane, through the peptidoglycan layer through to the outer membrane of the cell.
This project utilized multi-disciplinary techniques to express, purify and begin characterization of the BcsE protein. This will lead to information on the secondary structure and 3-D shape of the protein, as well as active site architecture and putative binding sites. Functional studies can also be started. These include enzyme assays and knock-outs studies to determine the effect of the absence of the protein on the ability of bacteria, specifically *E. coli*, to produce cellulose.
Understanding the process with which bacterial cellulose is produced and exported, can give insight into novel methods to combat prolonged infections due to the presence of biofilms. The information gathered from this project can form a basic model of how other exopolysaccharides, relating to biofilms, are produced in bacterial species.

95 16:20 Saturday BSB-136

Hisactophilin: The Adventures of the Truncation Mutant, L76A E Tran <*tran.elisa7@gmail.com*>, **D MacKenzie** <*dwsmac@gmail.com*> and **E Meiering** <*meiering@uwaterloo.ca*>, Meiering Lab, University of Waterloo, 200 University Ave. W., Waterloo, Ontario, N2L 3G1.

Myristoylation, the covalent linkage of a C14 fatty acyl chain to the N-terminus of a protein, is a common modification that plays a critical role in many cellular processes. Hisactophilin is an example of one such protein that is modified with this hydrophobic moiety, in this case to reversibly anchor onto plasma and nuclear membranes to aid in cell structure, mobility, and osmotic stress in response to pH changes. The importance of myristoylation of hisactophilin has been recognized; however, the mechanism of myristoyl switching remains unclear. Previous experiments performed in the Meiering group have shown that myristoylation increases the rate of folding and unfolding in wild-type hisactophilin. Further, studies by the Meiering and the Levy groups have shown the involvement of nonnative interactions in the folding and switching of myristoylated hisactophilin. Nonnative interactions are interactions that are absent in the final folded state of the protein and are important in the folding pathway of proteins, but remain poorly understood by the scientific community. To further study these nonnative interactions, hydrophobic truncation mutants were generated using coarse grained simulations. Here, the challenges associated with the expression, growth and purification of the truncation mutant, L76A, from E.coli, will be discussed in detail.

96 13:40 Saturday BSB-138

Investigating the dimerization interface in the RR protein VraR through a single point mutation. D. Golemi-Kotra <*dgkotra@yorku.ca*> and **V. Gagarina** <*gagarinavarvara@gmail.com*>, Department of Chemistry and Biology, York University, Toronto, ON, M3J 1P3.

VraSR Two-component system is a phosphotransfermediated signaling system implicated into vancomycin and β-lactam antibiotics resistance in *Staphylococcus aureus*. Upon antibiotic-associated cell wall damage, the histidine kinase VraS is subjected to ATP-dependent autophosphorylation at a conserved histidine (His) residue. Subsequently, phosphoryl group is transferred from VraS to the cognate response regulator VraR causing its transformation to biologically active form, a dimer. Previous studies have been shown that Mg^{2+}-dependant phosphorylation of Asp-55 on VraR receiver domain causes formation of new hydrogen bonds around the phosphorylation site with consequent repositioning of Thr-83 and Tyr-102 (classical T-Y coupling mechanism) that results in reorientation of the receiver domain and formation of α-1 dimerization interface. We introduce a point mutation into the position Met-13 (M13A) of the α-1 and demonstrate that this residue is critical for dimerization. Our findings show that the mutation at Met-13 completely abolishes formation of the dimer while the protein is able to undergo phosphorylation.

97 14:00 Saturday BSB-138

HDAC4 interaction with Myocyte Enhancer Factor 2 (MEF2) **R Aram** <*aramr88@yorku.ca*>, **Wales S., McDermot JC.** York University.

Myocyte Enhancer Factor 2 (MEF2) is a transcriptional activator involved in skeletal muscle development. Class IIa Histone Deacetylases (HDACs) interact with and directly suppress the transcriptional activity of MEF2 transcription factors. Kruppel-Like factor 6 (KLF6), a MEF2D target gene that is involved in growth and tumor suppression pathways. Previous research has shown that MEF2D may act as an activator or repressor of KLF6. The aim of this research was to understand how MEF2 may regulate the expression of KLF6 through HDAC4 in a myogenic context. The activity of HDAC4 was repressed using BML-210 and TSA drug treatments as well as with HDAC4 siRNA. Using a MEF2 reporter gene we determined that repression of HDAC4 indeed increases MEF2 transcriptional activity in C2C12 myoblasts. Additionally, the expression of a KLF6 reporter gene increased upon knockdown of HDAC4 however deletion of the MEF2 binding site showed no increase in KLF6 gene expression, suggesting MEF2 inhibits KLF6 expression in an HDAC4 dependent manner.

98 14:20 Saturday BSB-138

Structural and Functional Analysis of the Bcs C protein from the Bacterial Cellulose Protein Complex in Escherichia coli **J.P. Skrinjaric** <*skri0130@mylaurier.ca*>, **R Slawson** <*rslawson@wlu.ca*>, **G Horsman** <*ghorsman@wlu.ca*> and **J.T. Weadge** <*jweadge@wlu.ca*>, Wilfrid Laurier University, 75 University Ave W , Waterloo, ON , N2L 3C5.

Many persistent and chronic bacterial infections, especially those involving Escherichia sp., can be attributed to their ability to produce a biofilm. Biofilms can be described as a community of bacterial cells living within a self-produced, hydrated polymeric matrix, facilitating adherence to surfaces and confering benefits for the bacteria. In order to produce and export the biofilm, the bacterial cellulose synthase complex, composed of several different proteins, is utilized. One of these proteins is Bacterial Cellulose Synthase C (BcsC), which exhibits significant homology with the alginate secretion system of Pseudomonas aeruginosa. This system has been shown to guide the internally synthesized polymer to the outer membrane and export it, using a β-barrel motif.To determine the structure and function of the BcsC protein, the protein can be subdivided into 3 gene constructs, each of which were recombined into plasmids. This allowed for large scale expression and purification of the individual proteins. It is hypothesized that the β-barrel domain will be expressed in the insoluble cell fraction, because it is a membrane protein, and must therefore be purified under denaturing conditions to separate the protein from other insoluble cellular elements. Crystallization trials, functional and folding assays will then be conducted to determine the relationship between structure and function. With an understanding of how these biofilm exopolysaccharides are synthesized and exported, methods to potentially hinder their formation and persistence may be developed.

99 14:40 Saturday BSB-138

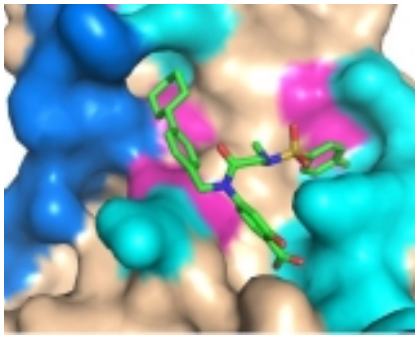
Docking Study on Giardia Flavohemoglobin **M. Eisner** <*me09fu@brocku.ca*> and **H. Gordon** <*hgordon@brocku.ca*>, Department of Chemistry, Brock University, St. Catharines, ON L2S 3A1; **J. Yee** <*jyee@trentu.ca*>, Department of Biology, Trent University, Peterborough, ON K9J 7B8; **S. Rafferty** <*srafferty@trentu.ca*>, Department of Chemistry, Trent University, Peterborough, ON K9J 7B8.

Giardia lambia is a parasitic protozoan that causes an infection in the small intestine; this is also known as traveller's diarrhea. Due to its living conditions, it is anaerobic and gets its energy from substrate-level phosphorylation, but can consume molecular oxygen.
Our collaborators Steven Rafferty and Janet Yee found a protein, Giardia Heme Protein 2 (gHBP2) that resembles the cytochrome b5 superfamily but has no known three dimensional structure. Although gHBP2 has been found, through spectrotroscopic titrations, to bind heme in a 1:1 ratio,1 and prossesses sequence similarity to cytochrome b5, it does not possess the histidines known to bind heme Fe2+ via axial coordination. Furthermore, giardia does not possess the proteins to synthesize heme. To determine the putative binding residues of gHBP2, a three dimensional model was constructed using SWISS-MODEL. The objective of this project is to evaluate the quality of the three dimensional model, and to dock heme and other potential ligands to the protein.
(1) Rafferty, S.; Luu, B.; March, R. E.; Yee, J. Biochem. Biophys. Res. Commun. 2010, 399, 347-351.

100 15:20 Saturday BSB-138

Metabolic Optimization of Potent Small Molecule Inhibitors of Stat3 Dimerization **S. Mac** <*sm.mac@mail.utoronto.ca*>, **C.C. Arpin** <*carolynn.arpin@utoronto.ca*> and **P.T. Gunning** <*patrick.gunning@utoronto.ca*>, Department of Chemical and Physical Sciences, University of Toronto Mississauga.

Signal transducer and activator of transcription 3 (Stat3) proteins are abberantly upregulated in various human cancers such as pancreatic, ovarian, breast, prostate, leukemia and lymphoma. Previous work on small molecule inhibitors has yielded promising results interrupting phosphorylated Stat3 (pStat3) dimerization, ultimately downregulating the expression of transcription factors and anti-apoptotic proteins involved in cancer cells. The goal of this research is to metabolically optimize proven potent small molecule inhibitors of pStat3 proteins in pancreatic cancer cells, by introducing a variety of modified substituents. Competitive binding assays, cytotoxicity and metabolic assays such as Caco-2 cell line studies have been conducted to assess this new generation of compounds for their potency and metabolic stability.



101 15:40 Saturday BSB-138

The Effect of pH and Chemical Denaturants on the Structure and Metal Status of Anthrax Lethal Factor **J. Mapletoft** <*jp_mapletoft@laurentian.ca*> and **S. Siemann** <*ssiemann@laurentian.ca*>, Laurentian University, Department of Chemistry and Biochemistry, Sudbury, ON, P3E 2C6.

Anthrax toxin (AT), a three-protein exotoxin secreted by the *Bacillus anthracis*, is one of the major virulence factors of anthrax. AT is composed of protective antigen (PA) and two enzyme components; the edema factor (EF) and the lethal factor (LF). PA is a multifunctional protein which binds to LF and delivers it to the endosome. Once in the acidic endosome, PA forms a pore and promotes the translocation of LF into the cytosol of the host cell. Here LF, a zinc-dependent metalloprotease, promotes the cleavage of mitogen-activated protein kinase kinases (MAPKK). Previous studies have suggested that the translocation of LF through the PA pore requires unfolding of the enzyme because the pore is too small to accommodate the folded protein. What remains unclear is whether such unfolding leads to the dissociation of zinc from LF's active site.
In this study, the influence of pH and the chemical denaturant urea on the structure of LF and its metal status was investigated using intrinsic tryptophan fluorescence spectroscopy and quantitative metal chelation, respectively. We found that, at pH 5, the zinc ion is released from LF at low urea concentrations, correlating well with the unfolding of LF. In contrast, at pH 6 and 7, the release of zinc from LF was impaired even at urea concentrations where the enzyme was found to be in the unfolded state. This demonstrates a synergistic effect between pH and exposure to denaturant with respect to the dissociation of zinc from LF. As such, it is not inconceivable that the combination of endosomal acidification and PA-induced partial unfolding leads to the dissociation of LF's zinc ion in-vivo.

102 16:00 Saturday BSB-138

An investigation into the molecular mechanism of human uncoupling protein-2 anion and proton transport **JP Parker**, **T Hoang**[a,b], **T Matovic**[a,b], **MD Smith** and **M Jelokhani-Niaraki**, [a]Wilfrid Laurier University; [b]University of Guelph.

Human uncoupling protein-2 (UCP2) is a mitochondrial membrane protein with a role in many physiological conditions such as diabetes and chemotherapy resistance. It transports both protons (H^+) and anions and helps to limit the formation of reactive oxygen species. In this study we show that the amino acids Arg76 (R76) and Arg88 (R88) play a crucial role in UCP2 chloride (Cl^-) anion transport and that mutations of Arg96 (R96) and Lys104 (K104) increase UCP2 proton transport rates. Four mutant proteins, each with one of the above residues replaced with a glutamine (Q), and the wild-type (WT) UCP2 were recombinantly expressed in E. coli and reconstituted in lipid vesicles. Their structures and H^+ and Cl^- transport capabilities were then measured. R76Q and R88Q mutant proteins showed reduced Cl^- transport when compared with WT UCP2 and R96Q and K104Q showed increased H^+ transport when compared with WT UCP2. Circular dichroism and fluorescence spectroscopy revealed that R76Q and R88Q proteins had similar conformations to WT UCP2 while R96Q and K104Q mutations caused structural changes to the protein. This work sheds light on the transport mechanism of UCP2 anion transport and the importance of structure in UCP2 H^+ transport.

103 16:20 Saturday BSB-138

Analysis of DAHP Oxime as a Transition State Mimic of DAHP Synthase **F. To** <*tof2@mcmaster.ca*>, **N. Balachandran** <*balacn5@mcmaster.ca*> and **P. J. Berti** <*berti@mcmaster.ca*>, Berti Lab, McMaster University, Hamilton, ON, L8S 4L8.

3-Deoxy-D-*arabino*-heptulosonate 7-phosphate (DAHP) synthase, the first enzyme in the shikimate pathway, catalyzes the aldol-like condensation of phosphoenolpyruvate and D-erythrose 4-phosphate to produce DAHP and inorganic phosphate. DAHP oxime, a potent inhibitor of this enzyme, was designed using transition state (TS) mimicry, however its mechanism of binding is not yet understood. We employed the measurement of linear free energy relationships and pH dependence of inhibition to determine whether DAHP oxime binds as a TS mimic. If the inhibitor is a TS mimic, then any change in catalysis, reflected in k_{cat}/K_M, should equally affect inhibitor binding, reflected in K_i, giving a linear relationship between $\log(K_i)$ vs. $\log(K_M/k_{cat})$. A series of active site mutants gave a fairly linear plot, suggesting that this inhibitor binds through some of the same interactions as the TS. The ionization states of the inhibitor were then determined, and no significant differences were found between its pK_a's compared to the proposed TS. The pH dependence of inhibition was characterized and was found to be similar to the pH dependence of k_{cat}, indicating that changes to the ionization states of the same catalytic residues affect both inhibitor binding and catalysis similarly. Taken together, these results suggest that DAHP oxime binds to DAHP synthase as a mimic of the tetrahedral intermediate formed during the reaction.

104 13:40 Saturday BSB-137

Effects of Ammonium Bicarbonate on the Electrospray Ionization Mass Spectra of Proteins **J. Hedges** <*jhedges2@uwo.ca*>, **S. Vahidi** <*svahidi@uwo.ca*> and **L. Konermann** <*konerman@uwo.ca*>, University of Western Ontario.

For intact protein analyses under non-denaturing conditions by electrospray ionization (ESI) mass spectrometry (MS) it is often desirable to employ "volatile" salts such as ammonium acetate that do not interfere with the ionization process. Due to its much higher buffering capacity at near-neutral pH, ammonium bicarbonate is sometimes suggested as an alternative. Surprisingly, ammonium bicarbonate induces the formation of very high protein charge states under certain instrument conditions, an effect previously referred to as "electrothermal supercharging".[1] In this study a series of experiments designed to elucidate the mechanism behind this phenomenon are conducted. Heating of a bicarbonate solution causes bicarbonate to decompose, generating carbon dioxide gas bubbles. It is well documented that proteins will denature and adsorb to the surface of gas bubbles.[2] As a consequence, the denatured proteins gain a large number of charges during ESI. These results further the understanding of the complicated ionization process of ESI-MS.

1. Harry J. Sterling, H.J.; Cassou, C.A.; Susa, A.C.; Williams, E.R. *Electrothermal Supercharging of Proteins in Native Electrospray Ionization*. Anal. Chem. **2012**, 84, 3795-3801.
2. Clarkson, J.R.; Cui, Z.F.; Darton R.C. *Protein Denaturation in Foam II. Surface Activity and Conformational Change*. J. Colloid Interface Sci. **1999**, 215, 333-338.

105 14:00 Saturday BSB-137

Correlation of photobleaching, oxidation and metal induced fluorescence quenching of DNA-templated silver nanoclusters **K. Morishita** <*kmorishi@uwaterloo.ca*>, **J. MacLean**, **B. Liu**, **H. Jiang**[a,b] and **J. Liu** <*liujw@uwaterloo.ca*>, [a]Department of Chemistry and Waterloo Institute for Nanotechnology, University of Waterloo, 200 University Avenue W, Waterloo, ON, N2L 3G1; [b]State Key Laboratory of Bioelectronics (Chien-Shiung Wu Laboratory), Southeast University, Nanjing 210096, China.

Few-atom noble metal nanoclusters have attracted a lot of interest due to their potential applications in biosensor development, imaging and catalysis. DNA-templated silver nanoclusters (AgNCs) are of particular interest as different emission colors can be obtained by changing the DNA sequence. A popular analytical application is fluorescence quenching by Hg^{2+}, where $d^{10}d^{10}$ metallophilic interaction has often been proposed for associating Hg^{2+} with nanoclusters. However, it cannot explain the lack of response to other d^{10} ions such as Zn^{2+} and Cd^{2+}. In our effort to elucidate the quenching mechanism, we studied a total of eight AgNCs prepared by dierent hairpin DNA sequences; they showed different sensitivity to Hg^{2+}, and DNA with a larger cytosine loop size produced more sensitive AgNCs. In all the cases, samples strongly quenched by Hg^{2+} were also more easily photobleached. Light of shorter wavelengths bleached AgNCs more potently, and photobleached samples can be recovered by $NaBH_4$. Strong fluorescence quenching was also observed with high redox potential metal ions such as Ag^{+}, Au^{3+}, Cu^{2+} and Hg^{2+}, but not with low redox potential ions. Such metal induced quenching cannot be recovered by $NaBH_4$. Electronic absorption and mass spectrometry studies offered further insights into the oxidation reaction. Our results correlate many important experimental observations and will fuel the further growth of this field.

106 14:20 Saturday BSB-137

Expanded Newborn Screening with Chemical Derivatization by MS/MS **M. Saoi** <*saoime@mcmaster.ca*> and **P. Britz-McKibbin** <*britz@mcmaster.ca*>, Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON.

The objective of this project is to develop a new chemical derivatization strategy under ambient conditions for rapid yet quantitative labeling of L-thyroxine (T4) and biocytin that represent specific biomarkers for congenital hypothyroidism and biotinidase deficiency, respectively. A ternary covalent chemical reaction based on base-catalyzed isoindole formation using either ortho-phtalaldehyde (OPA) or naphthalene dialdehyde (NDA) in conjunction with thiocholine as a novel cationic thiol co-reagent was developed. Rigorous optimization of the derivatization conditions was performed by UV-Vis absorbance spectroscopy, capillary electrophoresis and electrospray ionization-mass spectrometry (ESI-MS). Preliminary results indicate that the reaction allows for quantitative labeling of both T4 and biocytin under mild/weakly alkaline conditions in most cases under 5 min. The impact of buffer pH, organic modifier, dialdehyde reagent and amino acid substituent were also examined when using trimethylamine as non-reactive buffer. MS/MS together with chemical derivatization provides a simple way to enhance ionization efficiency needed for reliable quantification of nanomolar levels of labile metabolites in complex biological fluids.

107 14:40 Saturday BSB-137

Paper Based Solid-Phase QD-FRET Nucleic Acid Hybridization Assay **A Shahmuradyan** <*anna.shahmuradyan@mail.utoronto.ca*>, **O. M. Noor** <*omair.noor@utoronto.ca*> and **U. J. Krull** <*ulrich.krull@utoronto.ca*>, Chemical Sensors Lab, University of Toronto,, Mississauga, ON.

A paper based solid-phase nucleic hybridization assay has been developed. The method implements fluorescence resonance energy transfer (FRET) from immobilized quantum dots (QDs) to molecular dyes that are associated with hybrid formation on the QDs as means of signal transduction. The surface of the cellulose based paper was modified and functionalized with imidazole groups in order to facilitate immobilization of the glutathione-capped QD-probe oligonucleotide conjugates that were assembled in solution. The target oligonucleotides were labeled with Cy3 which acted as an acceptor of the energy emitted from the green QDs. The target oligonucleotides were labeled with the dye at the 3' end to ensure proximity for efficient energy transfer. The FRET-sensitized emission intensity form the Cy3 served as the analytical signal. The quantitative response of the assay was demonstrated by developing a calibration curve with fully complementary target. Without any amplification steps, the limit of detection was found to be 300 fmol with an upper limit of 5pmol. The selectivity of the assay was demonstrated by single-nucleotide polymorphism (SNP) detection, and the contrast ratio was determined to be 19 to 1.

108 15:20 Saturday BSB-137

Rapid time-scale dynamics and structure of Abeta(1-40) interacting with micelles **S. Tawadrous** <*saratawa@yorku.ca*>, The Wilson Group, York University, 4700 Keele Street, Toronto, Ontario, M3J 1P3.

Interactions between amyloidogenic proteins and membranes are widely thought to be an important factor in the onset of Alzheimer's disease (AD). β-amyloid peptide exists in two forms in the brain; the longer 42 residue β(1-42) which dominates the plaque deposits and the shorter 40 residue β(1-40) which is produced in higher proportions in the brains of people with AD. This study uses H/D exchange on a microfluidic device and time resolved ESI-MS to capture the millisecond-to-second interaction of the amyloid-β peptide with n-Dodecyl-β-D-maltoside (DDM) at a concentration well above the critical micelle concentration. In this membrane modeling environment, the peptide exhibits lower protection factors between residues 10 and 17 which are likely solvated by water, and higher protection factors near the C-terminal between residues 20 and 34, likely due to a specific interaction with the DDM micelles. Using the same device, HDX was performed on the soluble monomer β(1-40) in DMSO at pH 7.08 and exhibited a largely unstructured deuterium profile with uniformly low protection factors. The structural analysis herein confirms a stabilizing interaction between β(1-40) and monolayer micelles occurring primarily near the C-terminus. These results have influence in the therapeutic design of inhibitors and the determination of the repercussions of membrane integrity to subsequent brain atrophy.

109 15:40 Saturday BSB-137

Methods for small-volume analysis of phosphopeptides using magnetic beads **A. A. Thompson** <*athom28@uwo.ca*> and **K. K. C. Yeung** <*kyeung@uwo.ca*>, Department of Chemistry , The University of Western Ontario.

Abstract
The detection and analysis of phosphorylated proteins and peptides plays a significant role in understanding a wide range of cellular processes. Phosphopeptides often go undetected in Mass Spectrometry (MS) analysis due to both their acidic nature and sometimes due to a low ratio of phosphorylated peptides to unphosphorylated peptides. Often, Immobilized Metal Affinity Chromatography (IMAC) is used to selectively isolate phosphopeptides from small-volume samples, removing basic peptides that would be ionized in MS more readily than the phosphopeptides and solving the problem of low abundance. These techniques are successful in-vial with microliter samples but nanoliter sample volumes provide a new challenge due to limitations of micropipettes, solvent evaporation, and sample loss. This study investigates the miniaturization of phosphopeptide detection strategies using capillaries small enough in diameter to handle sub-microliter volumes and the injection of IMAC magnetic beads from an external droplet. IMAC magnetic beads can be easily manipulated in capillary using an external magnet to form a plug, allowing in-capillary solid phase extraction. The extraction effectiveness of three different IMAC beads are compared, 37-100µm iron-oxide coated beads, 5µm iron oxide coated beads, and 1µm non-magnetic titanium dioxide coated beads. A method of injection from an external droplet of magnetic beads is investigated and problems with this technique are discussed. The use of a droplet of solution to recover peptides dried on the tip of a capillary was tested at various lengths of time. Injections of 5µm diameter beads were successful and reproducible; however these beads were not

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Development towards a semi-quantitative paper-based immunoassay for eosinophil peroxidase. **K Yin** <*yinkr@mcmaster.ca*>, **C Sicard** <*clemence.sicard@gmail.com*> and **JD Brennan** <*brennanj@mcmaster.ca*>, .

Serious respiratory diseases such as asthma and pneumonia are relatively commonplace within the Canadian population. However, in clinical settings it is often difficult to accurately diagnose the root causes of respiratory distress. Asthma is an immune-driven inflammation requiring corticosteroids, while influenza and pneumonia are infections requiring antibiotics or antivirals. Since these two classes present with similar symptoms, there exists a need for a rapid and specific diagnostic test to differentially diagnose the causes. The current method of obtaining patient history and spirometry measurements are incapable of accurately determining the cause of respiratory distress. Point-of-care paper based analytical device are able to generate rapid and accurate results requiring minimal equipment. This provides the optimal platform for developing a diagnostic bioassay.

High levels of eosinophils (white blood cells) have been linked to immune-driven inflammation. An ELISA for eosinophil peroxidase (a protein biomarker for eosinophils) and a device for rapidly purifying protein from induce sputum are both commercially available. This work aims to develop a paper-based assay capable of semi-quantitatively determining the levels of eosinophil peroxidase from an induced sputum sample. The project's current progress is a drop applied ELISA on paper using gold nanoparticles as the generated signal.

111 16:20 Saturday BSB-137

Synthesis and testing of an activity-based elemental tag for *O*-GlcNAcase **M.A. Lumba**, **P. Cao** and **M. Nitz** <*mnitz@chem.utoronto.ca*>, Department of Chemistry, University of Toronto, Toronto, Ontario, M5S 3H6.

Activity-based probes are employed to specifically label enzymes on the basis of the enzymatic activities of the proteins. This technique not only reports the expression level of an enzyme but also offers insight into its catalytic activity. Labelled enzymes are traditionally detected by probes bearing a fluorophore. However, measuring fluorescence restricts the number of different enzymes one could detect simultaneously in a given sample, due to spectral overlap of fluorescent emission. To overcome this challenge, elemental tags with well-resolved mass signals are used to label enzymes, with detection by inductively coupled plasma mass spectrometry (ICP-MS). The lanthanides are an excellent choice of mass tags for biological applications, as they are of low abundance *in vivo* and possess a number of stable isotopes. We are interested in studying the protein, *O*-GlcNAcase, an enzyme that cleaves *O*-linked *N*-acetylglucosamine (O-GlcNAc) residues off proteins and is implicated in the aetiology of Alzheimer's disease, type II diabetes and cancer. An activity-based elemental tag was synthesized and tested *in vitro* using an inhibition assay. The probe competes with the enzyme's native substrate and delivers the metal tags, a result verified by ICP-MS. Multiplexed experiments and *in vivo* studies in Jurkat cells will soon be undertaken. This approach has great potential for applications in clinical studies, particularly in the early detection of disease.

112 13:40 Saturday BSB-115

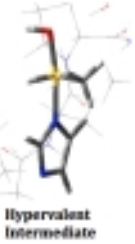
An Evaluation of Regions of Flexibility in the F-Spondin Reeler Domain Using Molecular Dynamics Simulations **K Stromski** <*ks00bl@brocku.ca*>, **A Madarati** and **H Gordon** <*hgordon@brocku.ca*>, Brock University, Department of Chemistry, St. Catharines, ON L2S 3A1.

F-spondin is a secreted extracellular membrane protein implicated in axonal growth. It consists of eight separate domains including the reeler domain, named so based on its homology to another extracellular matrix protein: reelin. X-ray crystallography experiments by Nagae et al.[1] produced a 3D β sandwich structure consisting of nine beta strands divided into 4 and 5 stranded anti-parallel beta sheets. The N-terminal end of the reeler domain includes a long flexible loop between a disulfide bridge and the start of the first beta strand. This loop wraps around the center of the beta sandwich motif. The region was termed the loose belt by Nagae et al. and was hypothesized to have a possible function in mediating protein-protein interactions.[1]
To evaluate flexibility of the loose belt under solvated conditions, molecular dynamics simulations (MDS) were performed. Starting from three different crystallographic conformations and solvated by a truncated octahedron of explicit water molecules, MDS were run for a total of 8 ns using nano-scale molecular dynamics (NAMD). Dihedral principal component analysis of each simulation identified the same two regions, one being the loose belt, associated with the greatest amount of flexibility within the protein. The results from our investigation will be presented and discussed.

1 Nagae, M.; Nishikawa, K.; Yasui, N.; Yamasaki, M.; Nogi, T.; Takagi, J. *Acta Crystallographica Section D: Biological Crystallography* **2008**, *64*, 1138.

113 14:00 Saturday BSB-115

Reduction of Hydrogen Peroxide via Archaeal Thioredoxin Peroxidase: A Mechanistic DFT Investigation **D.J. Simard** <*simardd@uwindsor.ca*>, **H. Dokainish** <*dokaini@uwindsor.ca*> and **J.W. Gauld** <*gauld@uwindsor.ca*>, University of Windsor.



High concentrations of reactive oxygen species (ROS) are hazardous to cells as it contributes to various diseases, cancers and is suggested to play a key role in aging. Consequently, reducing oxidative stress is a continuous task for all forms of life. Fortunately, there exist ubiquitous enzyme antioxidants such as peroxiredoxins (Prx) that are able to reduce ROS such as hydrogen peroxide at rates in the order of 10^6 M^{-1} s^{-1}. A specific Prx known as Archaeal Thioredoxin Peroxidase (ApTPx) in the species Aeropyrum pernix K1 was recently shown to have a histidine in its active site that may play a new role in catalysis by forming a hypervalent sulfurane intermediate. In general, hypervalent intermediates are not commonly formed in biological systems. Thus, in order to understand how this enzyme functions, an assessment was performed to determine a level of theory that can appropriately model this system. Furthermore, a quantum mechanical cluster approach was used to examine mechanistic details of hydrogen peroxide reduction by ApTPx, including formation of the hypervalent compound. Results from this study will be presented.

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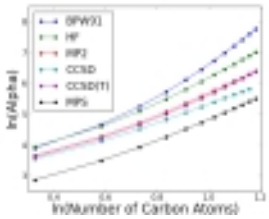
Polarizability Calculations of Linearly Conjugated Systems Using Matrix Product States **T. Kim** <*kimt33@mcmaster.ca*>, **P. Limacher** and **P. Ayers**, Department of Chemistry and Chemical Biology, McMaster University, Hamilton, Ontario, Canada; **S. Wouters** and **D.V. Neck**, 2Center for Molecular Modelling, Ghent University, Ghent, Belgium.



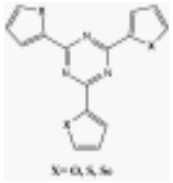
The matrix product state (MPS) method recently implemented by Wouters et al. (1) is used to determine the static polarizability and second hyperpolarizability of polyene chains with a fully active π orbital space. Comparison of various active spaces revealed that the contribution of the active σ orbitals is less significant than that of the π orbitals and thus can be neglected. The polarizabilities of polyene systems ranging up to 21 double bonds were calculated with the finite field method using different basis sets and can now be used as an accurate benchmark for other ab initio methods (See Figure). These results demonstrate for the first time that the benefits of MPS, well studied for small model systems, can be efficiently transferred to real chemical systems of substantial size.

Reference
1. Wouters, S.; Limacher, P. A.; Neck, D.V.; Ayers, P.W. Longitudinal static optical properties of hydrogen chains: Finite field extrapolations of matrix product state calculations. J. Chem. Phys. 2012, 136, 134110.

115 14:40 Saturday BSB-115

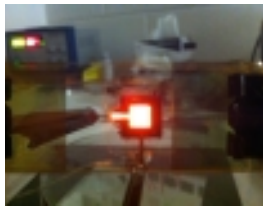
Electronic Properties of Probed Polyaromatic Heterocycles by DFT Calculations **O. Beiraghi** <*beiragh@uwindsor.ca*>, **S.H. Eichhorn** <*eichhorn@uwindsor.ca*> and **J.W. Gauld** <*gauld@uwindsor.ca*>, University of Windsor.

Our overall objective is to develop side-chain free columnar discotic liquid crystals to enhance the electronic interactions between the individual semiconducting columnar stacks and, subsequently, their overall performance as semiconductors. Presented here are results of DFT calculations using B3LYP method using varying basis sets we employ as a predictive tool for molecular properties to single out the most promising compounds as synthetic targets. Molecular properties we calculate and compare are lowest energy conformations, frontier orbital energies and topologies, and polarizability. The use of heavier heteroatoms in the shown triazine derivatives, for example, clearly lowered their HOMO-LUMO gap and increased their polarizability. However, we limit our choice of molecules to those structures that can be expected to be thermally stable (>200 ºC) in air.



116 15:20 Saturday BSB-115

Liquid Metal for use as Dynamic Electrode in Intrinsically Stretchable Devices **P. J. Prochazka** <*prochazp@uwindsor.ca*>, **S Amyotte** <*amyotte@uwindsor.ca*> and **T. B. Carmichael** <*tbcarmic@uwindsor.ca*>, University of Windsor.



This research project uses new innovative techniques to fabricate fully encapsulated, stretchable light emitting electrochemical cells (LEEC) that demonstrate large area light emission and tolerate linear stretching of up to 18%. This process utilizes the fabrication of a stretchable gold semi-transparent anode, followed by an evenly dispersed polymeric light-emitting layer and then the implementation of microfluidic channels of liquid metal as a cathode. These channels can be fabricated by casting polydimethylsiloxane (PDMS) onto a patterned silicon master. Through plasma oxidation, the PDMS channels can be covalently bound directly to the underlying PDMS substrate, forming a single unit, stretchable, light-emitting device. The characterization of light emitting devices via photomicrographs as well as external quantum efficiency and elongation at failure measurements were implemented. Some results will be presented.

117 15:40 Saturday BSB-115

The Electrochemical Monitoring of the Degradation Process of Fuel Cell Catalysts using Electrochemical Impedance Spectroscopy **O. Reid** <*Orian.Reid@uoit.net*>, **F.S. Saleh** <*Farhana.Saleh@uoit.ca*> and **E.B Easton** <*Brad.Easton@uoit.ca*>, University of Ontario Institute of Technology, 2000 Simcoe Street North Oshawa, Ontario, Canada L1H 7K4.

Proton exchange membrane fuel cells (PEMFC) use hydrogen and oxygen gas as a fuel source, and are a promising alternative for a new sustainable energy source with its many applications. The different components that make up the fuel cell all play a crucial role in performance, but the catalyst layer is the most expensive component because of the precious metal catalyst which in most cases is Platinum. Finding an easy way to monitor the degradation of the catalyst over time can give a better understanding of the different Pt degradation mechanisms, and also allow catalysts to be made that will have longer life times for different applications. Recently we have used an accelerated degradation testing protocol (ADTP) to monitor the degradation of the catalyst support through in-situ half-cell testing using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). For this project we have looked at using the same ADTP to monitor the degradation of the whole catalyst layer through in-situ full cell testing. We have advanced the testing protocol by conducting EIS at different DC bias potentials. This will allow the resolution of different Pt degradation processes, such as Ostwald ripening and Pt dissolution from carbon corrosion, to be observed. The data collected showed a linear correlation between the electrochemically active surface area (ECSA) and impedance at each potential. This information can be used as a method to determine the ECSA of a catalyst without the use of cyclic voltammetry.

118 16:00 Saturday BSB-115

Understanding and Preparation of Sharp Metallic Tips Via Electrochemical Etching **A. Awez Mohammad** <*awezmoa@mcmaster.ca*>, **Y. Wang** <*wang263@mcmaster.ca*> and **P. Kruse** <*pkruse@mcmaster.ca*>, Department of Chemistry and Chemical Biology, McMaster University.

Preparation of sharp probes has played an important role in nanotechnology. Most common methods of fabrication include mechanical cutting, micro-crystalline growth and electrochemical etching. The latter method is the most reproducible, resulting in stable tips. Sharp tips from wires of metals, including W, Au, Pt, Ir, and Ni have been prepared. The safety of the etching procedure and the quality of the tips prepared could be significantly enhanced if a stronger emphasis was put on an understanding of the physical and chemical aspects of the tip etching process. The parameters and properties of the tip etching have been investigated. During tip etching, a thin viscous film heavier than the electrolyte flows down the wire due to a lack of adherence. The passive film aids in protection of the wire from anodic dissolution via diffusion-limited kinetics. The downward flow of the passive layer exposes the area of the wire near the electrolyte-air interface to higher dissolution rates due to a Plateau-Rayleigh instability. The selective etching at the meniscus leads to a necking of the wire whereby a tip is formed. Most recipes agreed with formation of a slipping passive layer comprising of anionic metal species (such as $[WO4]^{2-}$, $[AuCl4]^{2-}$, $[AgSO4]^{-}$, $[Co(EDTA)]^{2-}$, etc.) that are attracted to the anode. Disturbances such as oxygen bubbling, high currents and formation of a passive oxide layer prevent successful etching of the wires. Tips on the submicron scale of metals including Ag, Al, Co, Cu, Fe, In, Mo, Sn, Ti, Ta, V, and Zn have been prepared.

119 16:20 Saturday BSB-115

Electrochemical and Microscopic Investigation of the Corrosion Behaviour of Mg AM50 Alloy **W. J. Binns** <*wbinns@uwo.ca*>, **R. M. Asmussen** and **P. Jakupi**, Western University.

One of the largest problems facing the widespread adoption of electrical vehicles today is the relatively short range achieved per charge of the vehicle. One way to combat this issue is to drastically reduce the weight of vehicles while maintaining structural integrity. To this end, magnessium alloys have been suggested as a possible material due their high strength to weight ratio. If magnessium alloys are to be incorporated into automobiles it is imparative that their corrosion behaviour be understood in order to guarentee safety and good design.
The goal of this study is to investigate the corrosion behaviour of die cast, graphite cast, and sand cast MgAM50 alloys both electrochemically and microscopically. Each cast was investigated electrochemically via Corrosion Potential measurements, Potentiodynamic study, and Electrochemical Impedeance Spectroscopy. Each of the aformentioned experiments were conducted with varying electrolyte concentrations to determine the effect on corrosion behaviour. Additionally, the three casts were studied with Optical Microscopy, Scanning Electron Microscopy, and X-ray Photoelectron Spectroscopy in order to characterize the surface morphology before and after corrosion has taken place.

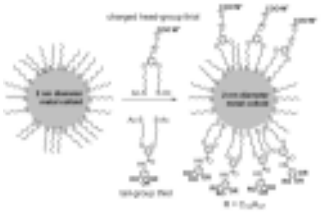
120 13:40 Saturday BSB-120

Controlling the Adsorption of DNA to Nanoceria **R. Pautler** <*repautle@uwaterloo.ca*>, **P. J-. J. Huang** <*p8huang@uwaterloo.ca*>, **J. Cao**, **B. Liu** and **J. Liu** <*liujw@uwaterloo.ca*>, Department of Chemistry and Waterloo Institute for Nanotechnology, University of Waterloo, 200 Univeristy Ave W, N2L 3G1.

The adsorption of DNA to nanoparticles has the potential for use in many fields including biochemical and catalytic applications. Cerium Oxide nanoparticles (nanoceria) have been relatively unstudied in this regard. Using FAM-labeled DNA it has been found that DNA length affects the adsorption to nanoceria while the sequence of the DNA seems to have no effect. The adsorption of DNA to nanoceria causes the fluorescence of the FAM-labeled DNA to be quenched allowing quantification of the amount of DNA that have adsorbed. The addition of buffer can affect the adsorption process; specifically citrate and phosphate buffer have been shown to both inhibit the adsorption process and cause the release of DNA after it has been adsorbed. The surface charge of nanoceria in solution with and without DNA has also been measured and it has been determined that the adsorption of DNA to nanoceria causes the surface charge to switch from positive to negative. These properties of the adsorption process have been used to control the oxidase-like ability of nanoceria to oxidize TMB. This research has the potential for many applications including the visual detection of DNA without a label down to a DNA concentration of 100 nM.

121 14:00 Saturday BSB-120

Synthesis and Characterization of Amphiphilic Nanoparticles **O. Zghal** <*zghal@uwindsor.ca*> and **S.H. Eichhorn** <*eichhorn@uwindsor.ca*>, University of Windsor, Windsor, ON, N9B 3P4.



The preparation of stable nano-sized colloids, or nanoparticles (NPs), is a field that has grown vastly over the past 10 years. Metal NPs are composed of a precious metal core and are usually between 1-100 nm in diameter. They can be coated with organic ligands containing various functional groups to give them different properties. Nanoparticle Surfactants (NPSs) are amphiphilic NPs that contain charged, polar head groups on one side and nonpolar, uncharged groups attached to opposite side of the NP. This transforms the NP into a charged, elongated, surfactant-like, amphiphilic structure that possesses self-organizing and self-assembling properties.
The objective of this project is to synthesize and investigate the properties of amphiphilic Au NPs. First, a hydrophobic ligand will need to be synthesized with long alkyl chains on one side of a rigid aromatic core and two thiol aliphatic groups on the other side. This hydrophobic ligand will be exchanged onto a gold nanoparticle coated with a monolayer of removable aliphatic thiols. A commercially available carboxyl aliphatic thiol will be subsequently attached and is expected to form a domain on the opposite side of the NPs when exposed to an interface. This will result in amphiphilic NPs for which the self-organization and assembly will be investigated by polarized optical microscopy and the Langmuir-Blodgett Method.

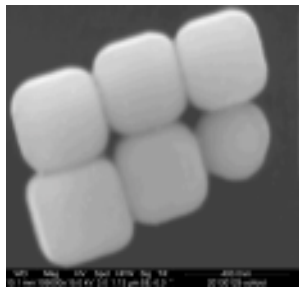
122 14:20 Saturday BSB-120

Shape Control in Noble Metal Nanoparticles: Silver Icosahedra and Gold Stars **R Keunen** <*keun4770@mylaurier.ca*>, **N Cathcart** <*cath9170@mylaurier.ca*>, **D Macoretta** <*maco3140@mylaurier.ca*> and **V Kitaev** <*vkitaev@wlu.ca*>, Wilfrid Laurier University, 75 University Ave. W, Waterloo, ON, N2L 3C5.

Noble metal nanoparticles (NP) display a variety of properties distinct from bulk materials that enable the realization of a large number of unique applications. As one of the noble metals, silver is commonly used to form a variety of nanoparticles because of its strong plasmon and a good balance of reactivity and stability that allows for the selection of certain particle morphologies. Silver icosahedral nanoparticles (AgI_hNPs) are nanoscale Platonic solids whose synthesis from pure silver has been elusive thus far.
We have developed a room-temperature synthesis of monodisperse AgI_hNPs using photochemical transformation in selective etching conditions. The light source is used to refine for silver nanoparticles that are generated using sodium borohydride as a reducing agent. Uniform AgI_hNPs form close packed arrays similar to spherical nanoparticles. We have also developed a synthesis for dendritic, gold star-like morphologies (stars) with icosahedral and octahedral core symmetries. This is a deceptively simple synthesis controlled by diffusion. The AgI_hNP arrays should be advantageous for potential applications in plasmonic sensing and surface-enhanced Raman scattering, SERS. The stars are promising for applications in plasmon sensing for biological assays.

123 14:40 Saturday BSB-120

Synthesis of shell isolated nanoparticles for plasmon enhanced spectroscopy **W Chen** <*chen112c@uwindsor.ca*> and **R Aroca** <*raroca1@cogeco.ca*>, Material and Surface Science Group,, University of Windsor, , 401 Sunset Avenue,, Windsor, Ontario, N9B 3P4, Canada.



The plasmonic enhancement of fluorescence and scattering is driven by the local field created in nanostructures of silver and gold that can sustain localized surface plasmon resonances (LSPR)1. The plasmon properties in nanostructures depend on their shape, size and the dielectric properties of the environment. Therefore, the fabrication of nanostructures with controlled plasmon properties is at the heart of practical applications. Here we report the chemical synthesis of silver and gold nanoparticles by reduction of silver and gold under special conditions to fabricate specific shapes, as those shown in the scanning electron microscopy image. The final goal is to develop reproducible protocols for the fabrication of the silver and gold metal nanostructures with well defined optical properties. Examples of plasmon enhancement of optical signals2 attained with these nanostructures are also discussed.

1. K. A. Willets and R. P. Van Duyne, Annual Review of Physical Chemistry, 2007, 58, 267-297.
2. R. Aroca, Surface-enhanced Vibrational Spectroscopy, John Wiley & Sons, Chichester, 2006.

124 15:20 Saturday BSB-120

Light-Activated Metal-Coordinated Supramolecular Complexes with Charge-Directed Self-Assembly **A Lopez** <*a3lopez@uwaterloo.ca*> and **J Liu** <*liujw@uwaterloo.ca*>, Department of Chemistry and Waterloo Institute for Nanotechnology, University of Waterloo.

Gold nanoclusters (AuNCs) and co-ordinated complexes have received significant attention in recent years. However, synthesis of fluorescent metal co-ordinated complexes has presented many challenges to overcome. Adenine and other related compounds have been in the past used to make metal co-ordinated complexes, although they have been non-fluorescent. In this work, we use a reduction method to acquire strongly fluorescent adenosine-Au, AMP-Au and ATP-Au complexes. Adenine only produced weak fluorescence, while cytidine, uridine and guanosine were non-fluorescent. The fluorescence of the complexes was at a wavelength of 470 nm for ATP and AMP and 480 nm for Adenosine and deoxyadenosine. Critical to the formation of fluorescent complexes were the addition of citrate and when it was added in the synthesis process, as well as the amount of exposure to light. Light exposure was seen as the largest contributor to the generation of fluorescence, as the complexes were only weakly fluorescent when left in the dark. In cases of adenosine and deoxyadenosine, micrometer sized particles were formed. However, when highly charged adenosine-rich species were used, such as ATP and AMP, the particle sizes were much smaller. In addition, the size of complexes was found to be controllable by mixing ATP and Adenosine in different ratios. This ability to change particle size, while preserving the same fluorescence can be used in many applications such as drug delivery, bio-sensing and imaging. This work was recently published in J. Phys. Chem. C (Anand Lopez and Juewen Liu, J. Phys. Chem. C, 2013, 117 (7), pp 3653-3661).

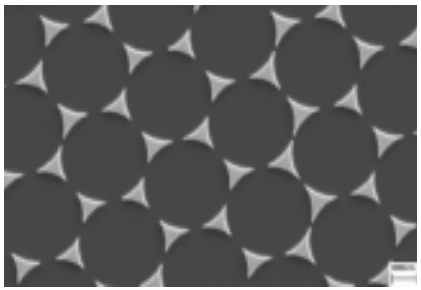
125 15:40 Saturday BSB-120

Photoelectrochemical Enhancement of $CuInS_2$ Light-Absorbing Layers for Solar Cells. **C. Hart** <*chart8@uwo.ca*>, **A. Tapley** <*atapley2@uwo.ca*> and **Z. Ding** <*zfding@uwo.ca*>, Department of Chemistry, The University of Western Ontario, 1151 Richmond Street, London, Ontario N6A 5B7.

The world is in need of low-cost renewable energy sources in order to compensate for the depletion of non-renewable fossil fuels. Solar cell technology can become more readily integrated for industrial use if their light-absorbing layers are cost effective to produce, with high photoconversion efficiency. Inorganic thin-film semiconducting materials such as copper indium disulfide ($CuInS_2$) could reduce the cost in the fabrication of solar in comparison to the typical silicon solar cells. A low-cost one-pot synthetic method for $CuInS_2$ nanocrystals (NCs) has been developed in our research group. We report herein on the photoelectrochemical (PEC) enhancement of our prepared $CuInS_2$ NC films by means of annealing and the addition of the n-type CdS buffer layer. During the optimization of these processes, PEC measurements were used to characterize the films without the need of making the full solar cell device. Methods such as scanning electron microscopy with energy dispersive spectroscopy, x-ray diffraction spectroscopy and intensity modulated photoelectrochemical spectroscopy were performed to investigate film compositions, topography and PEC mechanisms. Due to the use of a short capping ligand in the one-pot synthesis, a low temperature annealing method is proposed for the $CuInS_2$ NC films, generating an enhanced photocurrent response. Furthermore, an unusual approach of low temperature annealing of $CuInS_2$/CdS on ITO-glass proves to provide a greatly enhanced photocurrent density as high as 8.5 times the unaltered $CuInS_2$.

126 16:00 Saturday BSB-120

Determining the Limit of Detection of a Platform Fabricated by Nanosphere Lithography Used for Surface-Enhanced Raman Spectroscopy **G Wallace**, **M Tabatabaei** and **F Lagugné-Labarthet***, Department of Chemistry, The University of Western Ontario, 1151 Richmond Street, London ON, N6G 1Z1, Canada.



Substrates used for surface-enhanced spectroscopies such as surface-enhanced Raman scattering (SERS) or surface enhanced fluorescence (SEF) are of great interest for the detection of molecules at very low concentrations such as monolayers or isolated single molecules.
We report surface enhanced Raman spectroscopy measurements of molecules adsorbed on nanotriangle arrays made by nanosphere lithography. In order to determine the limit of detection of such platforms, solutions of 4-nitrothiophenol (4-NTP) were made with concentrations ranging from 1 mM to 1 aM. The solutions were exposed to the substrates for 24 hours and were probed under the exact same conditions and the limit of detection of 4-NTP was determined. A study trying to determine the limit of detection of Ochratoxin A, a food commodities toxin, was performed. In addition, parameters such as functionalization time and annealing of the sample prior to functionalization were investigated.

127 16:20 Saturday BSB-120

^{35}Cl SSNMR of HCl Pharmaceuticals: Pills, Polymorphs and Pure Forms **A.M. Namespetra**, **A.R. Sandre**, **K.J. Harris**, **M.P Hildebrand** and **R.W. Schurko**, University of Windsor, 401 Sunset Avenue, Windsor, ON, N9B 3P4.

Earlier work from our research group has demonstrated that ^{35}Cl solid-state NMR (SSNMR) is a powerful technique for the structural characterization of HCl active pharmaceutical ingredients (APIs) and the differentiation of polymorphs.[1,2] To date, ^{35}Cl SSNMR studies on HCl pharmaceuticals have focused primarily APIs in their pure forms. By investigating APIs in their dosage forms, it is possible to gain insight into the structures, arrangements, distributions and sizes of crystals within manufactured capsules and tablets. ^{35}Cl SSNMR is well suited for such investigations, and may even provide a possible routine screening method for quality and assurance.
To this end, I will present a systematic approach for the structural study of a variety of HCl pharmaceuticals in both pure and dosage forms using ^{35}Cl SSNMR (9.4 T and 21.1 T), powder X-Ray diffraction (pXRD), ^{13}C SSNMR and first-principles density functional theory (DFT) calculations. The combination of ^{35}Cl SSNMR data and DFT calculations allows the NMR parameters C_Q and η_Q to be determined for each crystallographically distinct chlorine site, providing insight into the local electronic environment and H-bonding network. Various acquisition techniques will be compared to develop a systematic and efficient approach to probing the dosage forms. In addition, it will be demonstrated that this method is capable of identifying polymorphic forms within capsules.
1. M.P. Hildebrand. (2012). *Solid-State NMR of Quadrupolar Nuclei for Structural Elucidation.* M.Sc. Thesis, University of Windsor, Canada. 2. H. Hamaed, J.M. Pawlowski, B.F.T. Cooper, R. Fu, S.H. Eichhorn and R.W. Schurko. *J. Am. Chem. Soc*. **2008**, *130*, 11056-11065.

128 13:40 Saturday BSB-119

Molecular Imaging of Cancer Using Dendritic Scaffolds **C. Colaneri** <*colanecj@mcmaster.ca*>, **L. Sadowski** <*sadowski@mcmaster.ca*> and **A. Adronov** <*adronov@mcmaster.ca*>, McMaster University.

In 2012, Prostate Cancer was the leading form of cancer among males with 26,500 new cases in Canada alone. Prostate specific membrane antigen (PSMA) is a membrane bound antigen which is over expressed in prostate tumour tissue making it a promising target for imaging. The coupling of a PSMA inhibitor to a bis-MPA dendrimer is explored as well as the coupling of a metal chelating ligand at the core. The multifunctional periphery of the dendrimer is expected to provide an advantage in the delivery of the inhibitor through the body. The core of the dendrimer will be radiolabeled to allow for a more accurate and location driven diagnosis of prostate cancer. Both generation 1 and generation 2 dendrimers will be synthesized in order to progress with future work in studying the effects of multivalency.

129 14:00 Saturday BSB-119

Selective Coating of T4 Bacteriophage through Controlled Silica Growth **J Kurian** <*kurianj@mcmaster.ca*>, **MA Brook** <*mabrook@mcmaster.ca*> and **MF Khan** <*madiha.fkhan@mcmaster.ca*>, McMaster University.

Model studies previously demonstrated that silica shells could be grown on polyvinyl pyrrolidone (PVP) using two different silica precursors, diglyceryl silane (DGS) or tetraethyl orthosilicate (TEOS). As the molecular weight of PVP increased, larger silica particles were observed indicating the ability to control silica growth. It was proposed that amide groups on PVP act as nucleation sites for silica. This concept was then applied to encapsulating T4 bacteriophages, which are also rich in amide groups. To determine the effect of silica growth on the bacteriophage, TEOS was employed as a precursor for silica. In order to control the rate of TEOS hydrolysis, hexane was added above the aqueous phase (containing bacteriophage) to limit TEOS diffusion into the aqueous layer. The effects of varying reaction time, TEOS concentration and the concentration of bacteriophage were examined using transmission electron microscopy (TEM). Selective coating of the phage head was observed. An increase in head diameter was observed after increasing TEOS and decreasing phage concentration, although no correlation with reaction time was observed. We have demonstrated the ability to selectively coat bacteriophages, which provides potential for these viruses to be used as effective biocontrol agents through their high specificity and efficiency in targeting bacteria.

130 14:20 Saturday BSB-119

Enzyme-mediated synthesis of siloxane-containing chiral polymers **J.P. Séguin** <*js09mz@brocku.ca*> and **P.M. Zelisko** <*pzelisko@brocku.ca*>, Brock University, Department of Chemistry and Centre for Biotechnology, 500 Glenridge Avenue, St. Catharines, ON, L2S 3A1.

Siloxane and chiral polymers individually have desirable physical and chemical properties which could be compounded if aspects of these two polymeric species were combined. Traditional polymerization chemistries such as radical, anionic, and cationic polymerizations are not typically stereoselective. Therefore, chirality is generally introduced into the polymers using chiral monomers. In the interest of developing "green" methodologies in silicon chemistry, we are developing a chemo-enzymatic method for synthesizing siloxane-containing chiral polymers. Immobilized lipase B from *Candida antarctica* (N435) is being explored as a potential biocatalyst to efficiently generate the disiloxane-containing chiral polymers from chiral diols and siloxane monomeric units. Several reaction conditions have been explored and an overview of the results will be presented.

131 14:40 Saturday BSB-119

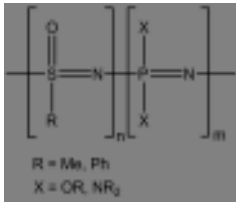
Thin Polymer Films as Cell Matrices **S.E. Sriskandha** <*sriskase@mcmaster.ca*>, **N.A.D. Burke** <*burken@mcmaster.ca*> and **H.D.H. Stover** <*stoverh@mcmaster.ca*>, McMaster University, 1280 Main Street West, Hamilton, Ontario.

There is great interest in the use of synthetic polymers as matrices for cell growth with applications in regenerative medicine, drug delivery and stem cell differentiation. The ability to modify the chemical and mechanical properties of the matrices is particularly desirable and provides an advantage over traditional biological supports.[1] This study focuses on the use of reactive hydrophilic polymers to prepare two-dimensional thin films for cell growth. A water soluble anionic copolymer poly(methacrylic acidco2-vinyl-4,4-dimethylazlactone) (PMV) was prepared through batch photopolymerization.[2] The azlactone group can rapidly react with amines to form crosslinked or functionalized films. Thin films were prepared through a layer-by-layer deposition technique of PMV and cationic poly(aminopropylmethacrylamide) (p(APM)) copolymers of varying APM content. Films were characterized to demonstrate crosslinking, and to determine the thickness, roughness and hydrophilicity. C2C12 myoblast cells were then seeded onto the thin films to test for cell attachment, viability and proliferation as a function of film properties.

1. M.E. Buck, D.M. Lynn, *Langmuir,* **2010,** *26(20)*, 16134-16140. 2. C. M. Gardner, H.D.H. Stover, *Macromolecules*, **2011**, *44,* 71157123.

132 15:20 Saturday BSB-119

A Controlled Synthesis of Polyoxothiazene-Polyphosphazene block-co-polymers **T Al-Faouri** <*tamara.alfaouri@ryerson.ca*>, **A.R McWilliams** <*amcwilli@ryerson.ca*> and **D.A Foucher** <*daniel.foucher@ryerson.ca*>, Ryerson University 350 Victoria Street Toronto, Ontario M5B 2K3.



The goal of this project is to carry out a controlled synthesis of polyoxothiazene-polyphosphazene block-co-polymers at ambient temperatures, through living polymerization process. These polymers are considered inorganic polymers with heteroatoms, other than the carbon, in their backbone which allows them to have various tuneable chemical and physical properties, with several applications such as fuel cell electrode membranes, catalysts, and chemical (oxygen) sensors. This project was approached by synthesizing the polyphosphazene block which can then be used as the initiator of the co-block polymerization after being added to the polyoxothiazene precursor at room temperature. This presentation will focus on the results from new approaches to the synthesis of polyoxothiazene precursors (including the use of ionic liquids) and the attempted copolymerization of phosphoranimines and sulfonimidoyl chlorides to form the target block copolymers.

133 15:40 Saturday BSB-119

Electrospun Conductive Nanofibres from Poly(ethylene oxide) Doped with Single-Walled Carbon Nanotube-Conjugated Polymer Constructs **F. Naeem** <*naeemf@mcmaster.ca*>, **A. Adronov** <*adronov@mcmaster.ca*> and **J. Moran-Mirabal** <*moran-mirabal@mcmaster.ca*>, Department of Chemistry and Chemical Biology, McMaster University, Hamilton, ON.

Electrospinning is a well-established technique for producing fibres in the micro- to nanometre scale through the application of a strong electric field to polymer solutions. These fibrous structures are attractive for integration within lab-on-a-chip devices due to their high surface area to volume ratio and ease of production. Furthermore, nanofibres are amenable to chemical surface modifications and can incorporate a range of chemical and biological structures within them, thereby allowing fabrication of nanofibres with tuneable properties.
This research involves electrospinning nanofibres from aqueous dispersions of poly(ethylene oxide) (PEO) and supramolecular constructs containing single-walled carbon nanotubes (SWCNT) that are functionalized with a conjugated polyelectrolyte (poly[2,5-bis(3-sulfonatopropoxy)-1,4- ethynylphenylene-alt-1,4-ethynylphenylene] sodium salt), which renders the complex water-soluble. The PEO serves to form a sufficiently viscous solution suitable for electrospinning and the SWCNT complex allows for the production of conductive nanofibres, which can be used for applications ranging from high surface area electrodes to tissue engineering scaffolds. However, prior to developing applications, it is important to optimize electrospinning parameters such as working distance and electric potential. Moreover, fibre morphology, conductivity, and SWCNT dispersion within the fibres must be characterized. In this presentation, I will discuss ongoing characterization of these nanofibres.

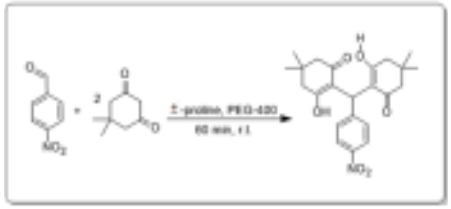
134 16:00 Saturday BSB-119

Stability of Aqueous Nanodroplets Containing RNA Complex **A. Malevanets**, **S. Constas** <*sconstas@uwoca*> and **M. Turnbull** <*mturnbu6@uwo.ca*>, Western University.

The study of charged macromolecules (macroion) in a droplet environment has far reaching uses in modern application. Mass spectrometry, electrospray ionization and deposition, and nanofluidics all function on the interactions of charged macroions and their droplet carrier. These interactions are highly complex, and require highly advanced computational codes and methods for their simulations. In this project, the complex interactions of the droplet and RNA were studied. Molecular simulations were performed for various sized droplets ranging from a few thousand, to tens of thousands of water molecules. These droplets were then put through an evaporation simulation. Past studies of poly(ethylene glycol) and polyhistidine indicated that the conventional charged residue model and ion-evaporation models do not hold for macromolecules in droplets ; rather, the macroion induces a charged stability greater than that predicited by Rayleigh stability. We see areas of highly ordered water molecules that remain un-evaporated for a long time. In this way, we observe 'spines' of water molecules forming off the macroion. These spines and induced stabilities constitute a unique environment for chemical reactions, and show a highly complex evaporation scheme that may have further electrospray and transportational uses.

135 16:20 Saturday BSB-119

Solvent Recyclability in the Undergraduate Organic Laboratory **A.P Dicks** and **J.M Stacey** <*jason.stacey@utoronto.ca*>, University of Toronto, Department of Chemistry.



Solvent recyclability is a fundamental industrial green practice that is commonly overlooked in the undergraduate laboratory curriculum. Here we describe two successfully-implemented third-year undergraduate experiments that highlight the principle of solvent recyclability to students. Polyethylene glycol (PEG) and glycerol are two "alternative" solvents that are readily recovered for reuse, either by students or the laboratory instructor. Glycerol is employed as the medium for sodium borohydride reductions as a procedurally simple display of recyclability. In addition, consecutive Knoevenagel and Michael condensations are performed that showcase recycling of PEG and racemic proline as an organocatalyst.
These reactions were both undertaken in third-year organic laboratories at the University of Toronto during 2012-13. Representative spectra and yield data will be presented based on results obtained by 60 students. Through emphasis of green chemistry at the undergraduate level, the education of future chemists will grow on a foundation that fosters appreciation for environmentally sound practices.

136 18:30 Saturday CIBC Hall (MUSC)

Microwave Assisted Functionalization of Water-Soluble, Size Separated Silicon Quantum Dots **K. Chen** <*kenny.chen@utoronto.ca*>, **M. Mastronardi** and **G. A. Ozin**, Department of Chemistry, University of Toronto.

Silicon nanocrystals (SiNC) have generated considerable attention as an environmentally abundant and non-toxic alternative to heavy metal chalcogenide based nanocrystals such as CdSe or CdTe. In particular, the synthesis of monodisperse and water-soluble SiNC remains a challenge and prerequisite to biomedical applications. To this end, we have developed a microwave-assisted method of surface functionalizing SiNC with carboxylic acids to produce SiNC that are colloidally stable at near neutral pH. The polydisperse samples can then be separated by size-selective precipitation and density gradient ultracentrifugation. With this technique we report a fast and effective way of producing relatively monodisperse water-soluble SiNC that display size-tunable photoluminescence. This progress takes us a step closer towards many opportunities including targeted cellular imaging, drug delivery and *in vivo* imaging.

137 18:30 Saturday CIBC Hall (MUSC)

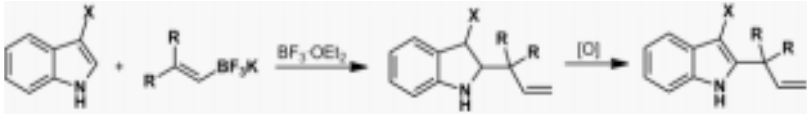
An Extended Study of the Effect of Betadine on Silicone Elastomers **T.R. Urlich** <*urlicht@mcmaster.ca*> and **M.A. Brook** <*mabrook@mcmaster.ca*>, Department of Chemistry and Chemical Biology, McMaster University.

Betadine is a topical antiseptic whose active ingredient is a polyvinylpyrrolidone-iodine (PVP-I) complex. The liberation of iodine from the complex exhibits an excellent range of antimicrobial activity while minimizing toxicity to humans, a pairing of characteristics that has made it the industry standard for over 60 years. Studies on the effect of Betadine on silicone breast implants have suggested that PVP-I oxidizes crosslinked silicones, leading to their degradation. The materials lose elasticity and become leathery or, in the worst cases, brittle. Following those reports, in 2000 the U.S. Food and Drug Administration suggested contact of Betadine with breast implants was contraindicated. Only a single report has tried to explain the origin of the chemical changes in radically cured implants. We have examined silicone elastomers cured by a variety of methods and will examine different degrees of change after exposure to Betadine, as a function of crosslink type. In addition, model studies with small functional silanes will allow us to speculate on the mechanisms of degradation.

138 18:30 Saturday CIBC Hall (MUSC)

Towards Allyation/Oxidation Protocols for C3 Functionalized Indoles with Potassium Organotrifluoroborates **P. Menzies** <*p.menzies@utoronto.ca*> and **R.A. Batey** <*rbatey@chem.utoronto.ca*>, University of Toronto, 80 St. George Street, Toronto, ON.

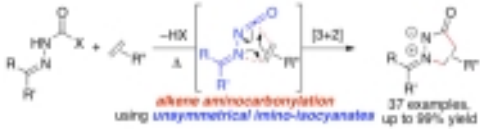
Organoboron compounds are known to be effective allylating reagents for aldehydes and imines. Allylboranes have recently been used to functionalize indoles at the relatively unreactive C2 position via the indole imine tautomer. However these reagents are challenging to make, sensitive and require extreme reaction conditions. Potassium organotrifluoroborate reagents have emerged as a promising alternative. These compounds are air stable and require milder reaction conditions. Allylations and prenylations of indole with these reagents have been successful, furnishing the corresponding 2,3-dihydroindole (indoline). It is desirable to perform these reactions on substituted indoles and to rearomatize the indoline to the corresponding indole. The resulting scaffolds are important intermediates in the total syntheses of many biologically active compounds. Allylations and prenylations of several substituted indoles are performed to determine the scope of organotrifluoroborate utility. Additionally, several oxidation conditions are screened to determine the best procedure by which to reform the indole nucleus.



139 18:30 Saturday CIBC Hall (MUSC)

A Simple Synthesis of β-Aminocarbonyl Compounds from Alkenes and Hydrazones **P. J. Moon** <*pmoon020@uottawa.ca*>, **W. Gan** <*weig1021@gmail.com*>, **C. Clavette** <*cclav076@uottawa.ca*>, **N. Das Neves** <*nicolas.dasneves@gmail.com*>, **T. Markiewicz** <*twdmarkiewicz@gmail.com*>, **A. Toderian** <*atode021@uottawa.ca*> and **A. M. Beauchemin** <*andre.beauchemin@uottawa.ca*>, Center for Catalysis Research and Innovation, Department of Chemistry, , University of Ottawa, 10 Marie Curie, Ottawa, Ontario, Canada, K1N 6N5.

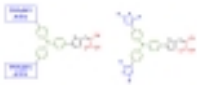
In recent years, peptidomimetics such as β-peptides have shown tremendous potential in medicinal chemistry. This unique class of compounds exhibits very interesting properties due to its non-natural β-aminocarbonyl backbone. This subunit is also very common in small-molecule pharmaceuticals and natural products. In an effort to develop novel amination methodologies, our group developed an efficient method to synthesize azomethine imines and β-aminocarbonyl compounds via the direct iminocarbonylation of alkenes (JACS 2012, 16111). Recent advances concerning the synthesis and reactivity of unsymmetrical azomethine imines will be presented.



140 18:30 Saturday CIBC Hall (MUSC)

The Synthesis of Modified Organic Dyes for Direct Integration into a Hole-Transport Material. **B Koivisto** <*oabdi@ryerson.ca*>, **O Abdi** <*devin.machin@ryerson.ca*> and **D Machin** <*bryan.koivisto@ryerson.ca*>, Ryerson University, 350 Victoria st, Toronto ON; **C Bonnier** <*c.bonnier@utoronto.ca*>, University of Toronto, Old Toronto, Toronto ON.

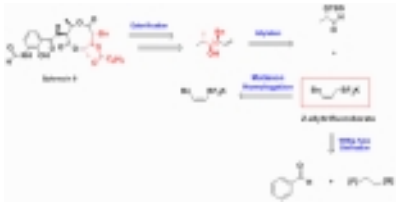
The dye-sensitized solar cell (DSSC) represents one of the most promising next-generation photovoltaic devices. The dye molecule is a key component in the DSSC; however, dye and device stability is limited through the use of corrosive liquid electrolytes. Replacing the liquid electrolytes with hole-transport materials should improve efficiency by increasing the kinetics of charge transfer and increase long-term device stability. Organic DSSC dyes are comprised of a redox-active donor/chromophore (i.e., triphenylamine) connected, through a conjugated linker, to an acceptor capable of anchoring to TiO2. In our hope to integrate dyes with polymeric HTMs, we have developed a family of dyes modified with polymerizable pendant arms that will directly integrate with the hole-transport material further increasing stability and regeneration rates. This paper will present the synthesis and physicochemical properties of triphenylamines modified with pendant arms as well as investigate their device efficiencies, prior to HTM integration.



141 18:30 Saturday CIBC Hall (MUSC)

Studies Toward a Wittig Olefination Route to γ-Functionalized Z-allyltrifluoroborates **D.A. Dalesandro** <*daniel.dalessandro@mail.utoronto.ca*>, **R.E. Beveridge** <*ramsay.beveridge@utoronto.ca*> and **R.A. Batey** <*rbatey@chem.utoronto.ca*>, University of Toronto, Department of Chemistry, 80 St. George Street, Toronto, Ontario.

Installing the key stereotriad in Splenocin 9 requires a specific Z-allyl trifluoroborate. Herein two approaches to the synthesis of this fragment are presented : a novel boronophosphonate two-pronged allylating agent, which could provide access to the Z-allyl trifluoroborate through a Wittig-type olefination followed by an allyl-boron addition, and the traditional approach based on work by Molander and Matteson which relies upon homologation of the corresponding Z-vinylboronate.



142 18:30 Saturday CIBC Hall (MUSC)

Synthesis and Self-assembly of PFS-b-PMMA Diblock Copolymers **K.X. Lin** <*kaixiang.lin@utoronto.ca*>, **M. Zhang** <*mezhang@chem.utoronto.ca*> and **M.A. Winnik** <*mwinnik@chem.utoronto.ca*>, University of Toronto , 80 St. George St.,, Toronto ON Canada , M5S 3H6.

Micelles formed by poly(ferrocenylsilane) (PFS) block copolymers in selective solvents are special. They form thin (15 nm), uniform rod-like structures for a broad range of polymer compositions. We believe that this shape is a consequence of the crystalline nature of the PFS core. Previous studies have focused on the self assembly of PFS-*b*-PI (PI = polyisoprene) and PFS-*b*-PS (PS = polystyrene) in non-polar solvents. I am interested in extending these studies to PFS-*b*-PMMA (PMMA=poly(methyl methacrylate)) block copolymers. Here, I can examine self-assembly in polar solvents like acetone and acetonitrile. In order to prepare a family of block copolymers with different PMMA chain lengths, I have designed a "click" chemistry approach. To proceed, atom transfer radical polymerization (ATRP) with an azide-functionalized initiator was used to prepare azide-end-capped PMMA polymers with narrow molecular weight distributions. Kinetic studies were carried out to determine the reaction temperature, time and monomer feed ratios needed to control the degree of polymerization. Subsequently, these azide-terminated PMMA chains were coupled to two samples of alkyne-terminated PFS through a copper-catalyzed azide-alkyne cycloaddition reaction. In this way, I prepared a library of PFS-*b*-PMMA block copolymers having different PMMA lengths. Preliminary results from self-assembly studies have shown that PFS_{54}-*b*-$PMMA_{141}$ formed fiber-like micelles with a PFS core and PMMA corona in ethyl acetate. In contrast, PFS_{26}-*b*-$PMMA_{224}$ did not form well-defined structures under these conditions. Further studies on these PFS block copolymers, with different length PMMA chains, should allow new insights into the self-assembly mechanism.

143 18:30 Saturday CIBC Hall (MUSC)

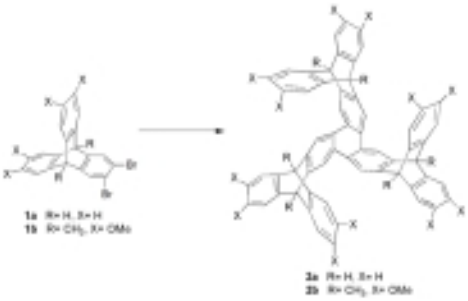
Controlling the wettability of acrylate polymers **Y. Chen** <*kaychenyq@gmail.com*> and **M.A. Brook**[a,b,c] <*mabrook@mcmaster.ca*>, [a]Department of Chemistry and Chemical biology; **M.F. Khan** <*madiha.fkhan@mcmaster.ca*>, [b]Department of Biomedical Engineering; **V. Delhorbe** <*virginie.delhorbe@gmail.com*>, [c]Department of Chemistry, McMaster University, Hamilton, ON, L8S1Y3.

As part of our studies on biomaterials, we wished to create surfaces with well-defined wettability using small silicone surfactants as constituents of acrylate polymer bodies. The silicone surfactants is comprised of an oligo(ethylene oxide) chain terminated at one end with a small silicone and at the other an acrylate. The content of the silicone surfactant was systematically varied in copolymerizations with methyl methacrylate. Polymerisations were undertaken thermally using AIBN as initiator, or under blue or UV light in the presence of camphorquinone. Random polymerization was compared with RAFT polymerization processes designed to create blocks.
Surprisingly, the water wettability did not relate linearly to the surfactant concentration. Instead, optimum wettability occurred near 60% surfactant: higher levels were associated with higher contact angles. The origins of the unusual wettability will be discussed.

144 18:30 Saturday CIBC Hall (MUSC)

The Synthesis of Heptiptycene Derivatives for Use in Host-Guest Chemistry **D.A.M. Ellis** and **K.E. Maly** <*kmaly@wlu.ca*>, Department of Chemistry, Wilfrid Laurier University, 75 University Ave. W., Waterloo, Ontario N2L 3C5, Canada.

Heptiptycenes are an area of interest because of their possible uses in host-guest chemistry. Their unique dual bowl-shaped cavities and rigid framework make them potential hosts for smaller electron deficient molecules such as TNT, cyanobenzene, nitrobenzene, and other aromatic compounds. The key steps in the proposed synthetic approach includes a benzyne formation followed by a Diels-Alder reaction with substituted anthracene to yield a substituted triptycene (**1**). This is followed by a palladium catalyzed aryne cyclotrimerization to give an extended heptiptycene (**2**). Our progress towards the synthesis of the target compound **2** will be presented.



145 18:30 Saturday CIBC Hall (MUSC)

Synthesis of Ferrocene-Cysteine Derivatives **Y.-C. Lin** <*yenchun.lin@mail.utoronto.ca*> and **H.-B. Kraatz** <*bernie.kraatz@utoronto.ca*>, University of Toronto.

Numerous metalloproteins discovered in biological systems require the existence of cysteine at the active site for the conjugation between the protein and metal ion. The thiol group of cysteine acts as a Lewis base to interact with metal ions.

In this research project, we are exploiting cysteine conjugates of ferrocene. The ferrocene acts not only as a scaffold to constrict the orientation of cysteine, but also as the redox center of the compound, which may allow monitoring of the metal-cysteine interaction by electrochemical means. The redox behavior of ferrocene changes as metal ion is coupled to cysteine. The goal of the project is to symmetrically synthesize a cysteine containing ferrocene derivative in solution phase. The redox behavior of ferrocene and the conjugation between cysteine and metal ion are studied through NMR and LCMS.

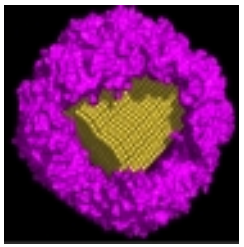
146 18:30 Saturday CIBC Hall (MUSC)

Deposition of Silver nanoparticles on cellulosic substrates for biomedical applications **C. Scott**, **J. Strap** and **L Trevani**, University of Ontario Institute of Technology.

Bacterial cellulose produced by Gluconacetobacter xylinus was impregnated with silver nanoparticles in situ by infusion with silver nitrate and ammonia to form the [Ag(NH3)2]+ complex, which was then reduced by varying concentrations of D-glucose in a Tollens type process. The formation and general size of silver nanoparticles was characterized by UV-Visible spectroscopy, scanning electron microscopy (SEM), and loading of silver nanoparticles was determined by thermogravimetric analysis (TGA). When the concentration of glucose relative to silver was increased, a shift in the visible spectrum absorption maximum was observed, indicating smaller particle size. The silver nanoparticle-impregnated cellulose was then dried by two different methods, either freeze-drying or vacuum drying, and the swelling behaviour of both methods was investigated. The cellulose dried by both methods were evaluated for antimicrobial properties against two different gram-negative organisms, Escherichia coli and Pseudomonas aeruginosa.

147 18:30 Saturday CIBC Hall (MUSC)

Controlled Encapsulation of Gold Nanoparticles by *Escherichia coli* Bacterioferritin **R. M. Taylor** <*rmtaylor@uwaterloo.ca*>, **A. van der Ven** <*a23vande@uwaterloo.ca*> and **J. Honek** <*jhonek@uwaterloo.ca*>, Honek Lab (ESC-244A), University of Waterloo, Waterloo, ON, N2L 3G1.



Escherichia coli bacterioferritin (Bfr) has been studied as to its ability to act as a host molecular framework for advanced bionanomaterials. The 24 subunit protein is natively utilized by *Escherichia coli* for iron storage, storing up to approximately 4500 iron atoms within its 8 nm internal cavity when fully filled. Our laboratory is developing methodologies to control the encapsulation of other molecular guests into this cage protein. Previous work in our laboratory has introduced Histidine (His) tags to the C-termini of the Bfr subunits by recombinant methods. The current research describes work done on utilizing this affinity tag to probe the limits of guest encapsulation within this protein by exploring the molecular encapsulation of various gold nanoparticles (GNPs), and to investigate the effects of encapsulation on GNP properties. These investigations utilized protein purification techniques such as size exclusion chromatography and a variety of biophysical techniques such as ultraviolet-visible spectroscopy and Transmission Electron Microscopy (TEM). Analysis of the experimental results confirmed the successful encapsulation of various GNPs within the internal cavity of Bfr and extends the capabilities of this protein framework to the area of bionanotechnology and advanced materials science.

148 18:30 Saturday CIBC Hall (MUSC)

Isolation and Purification of Voltage-Dependent Anion Channel (VDAC) in Mouse Myelin **MB Bhatia** <*bhat1660@mylaurier.ca*> and **L DeBruin** <*ldebruin@wlu.ca*>, Wilfrid Laurier University.

Myelin is the multi-layered plasma membrane that insulates the axon to ensure the rapid conduction of nerve impulses. Demyelination of the axons disrupts nerve impulse conduction, and progressively degenerates neurons. Consequences of demyelination are most evident through Multiple Sclerosis (MS). Voltage dependent anion channel (VDAC) has recently been identified as critical to the structure and function of the plasma membrane, through its role in apoptosis and demyelination, ion transport, and NADH:ferricyanide reductase activity. Therefore, this study aimed at (1) extracting and purifying VDAC from mouse myelin using 3% triton X-100 and diethylaminoethyl (DEAE) anion exchange chromatography, and (2) assessing the degree of purification of VDAC by measuring absorbance at 280nm, NADH:ferricyanide reductase activity, immunoblot and SDS-PAGE analysis. Absorbance at 280 nm and NADH:ferricyanide reductase assay showed peak activity for fractions eluted with high salt concentration buffer (250 mM NaCl). These fractions also showed presence of VDAC and Na+/K+ ATPase (a plasma membrane marker), indicating that VDAC contributed to the reductase activity and the total protein concentration in the eluted fractions. SDS-PAGE for the eluted fractions showed 30-35 kDa bands characteristic of VDAC, which was confirmed by Western blot analysis. It is interesting to note that several other fractions that did not show presence of VDAC in the immunoblot showed high reductase activity. This indicated the presence of other oxidoreductases that may also form a part of the trans-plasma membrane electron transport system. Upon purification, these enzymes can facilitate research on their involvement in demyelination and development of MS.

149 18:30 Saturday CIBC Hall (MUSC)

Interrogating p19-small RNA Interactions with Small Molecules **D.C. Danielson** <*Dana.Danielson@nrc-cnrc.gc.ca*> and **J.P. Pezacki**[a,b,c] <*John.Pezacki@nrc-cnrc.gc.ca*>, [a]Department of Biochemistry, Microbiology & Immunology, University of Ottawa; [b]National Research Council of Canada, Life Sciences Division; [c]Department of Chemistry, University of Ottawa; **R. Filip** <*rfili017@uottawa.ca*>, Faculty of Science, University of Ottawa.

The RNA interference pathway is present in a wide variety of organisms for endogenous gene regulation and is of particular importance in plants as a defensive mechanism against viruses. In this pathway, small RNAs are incorporated into the RNA-induced silencing complex (RISC) which then targets complementary transcripts and results in gene silencing. Certain viruses express proteins that function as suppressors of RNA silencing. Tombusviruses express the p19 protein to bind short interfering RNAs (siRNAs) with high affinity, preventing their incorporation into RISC. There have been recent advances in probing the RNA silencing pathway using small molecule inhibitors of the Argonaute protein, which is vital to the RISC complex. In this study, we explore whether three small molecules reported as inhibitors of Argonaute:siRNA interactions also inhibit p19:siRNA interactions in vitro. By performing electrophoretic mobility shift assays, we demonstrate that Aurintricarboxylic acid and Suramin both reversibly inhibit p19:siRNA binding with IC50 values of 0.43 and 430 μM, respectively, whereas Oxidopamine HCl does not inhibit p19:siRNA binding at the concentrations tested. Moreover, the differential binding affinities of Suramin for RISC and p19 suggests that p19 and Suramin may be used synergistically to suppress RNA silencing at two different points in the pathway. These results broaden our understanding of small molecule inhibition of protein:RNA interactions that may find application in probing the RNA silencing pathway in living systems.

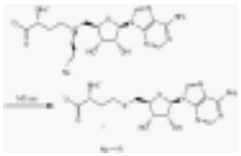
150 18:30 Saturday CIBC Hall (MUSC)

Soraphen A-Mediated Inhibition of Acetyl CoA Carboxylase Activity Represses Hepatitis C Replication **G Desrochers**, **R Singaravelu**, **P Srinivasan** and **J Pezacki**[a,b], [a]University of Ottawa; **S O'Hara**, [b]National Research Council.

Hepatitis C virus (HCV) is a major cause of liver disease world-wide, including hepatocellular carcinoma and hepatic steatosis. Hepatic steatosis is the by-product of the high cellular lipid levels required for the replication and proliferation of the hepatitis C virus. HCV induces increased intracellular lipid levels through upregulation of *de novo* lipogenesis and repression of lipid secretion and catabolism. The rate-limiting step of lipogenesis, the addition of carbon to acetyl-CoA to form malonyl-CoA, is catalysed by the enzyme acetyl-CoA carboxylase (ACC). It has been previously shown that Soraphen A (SorA) acts as a nanomolar inhibitor of acetyl-CoA carboxylase , and that is does so by preventing the polymerisation of long active ACC polymers from inactive dimers. Via luciferase assays, qRT-PCR and Western blot analyses, we have shown that SorA inhibits HCV replication in HCV cell culture models expressing subgenomic and full-length replicons (IC50 = 10 nM). Using coherent anti-Stokes Raman spectroscopy (CARS), a label-free method of imaging hepatic lipid content, we have shown that a higher concentration of SorA (100 nM) lowers the total cellular lipid volume in hepatoma cells. We are currently investigating the influence of HCV and SorA on ACC polymerization. Our results demonstrate that SorA is a valuable probe to study ACC's role in HCV pathogenesis.

151 18:30 Saturday CIBC Hall (MUSC)

Transfer of Chemical Moieties to Biomolecules Using S-Adenosyl-L-Methionine Dependent Methyl Transferases **TM Kay** <*tmkay@uwaterloo.ca*>, **CL Myers** <*cullen.myers@gmail.com*> and **JF Honek** <*jhonek@uwaterloo.ca*>, Honek Lab (ESC-244A), University of Waterloo, Waterloo, ON, N2L 3G1.



S-Adenosyl-L-methionine (AdoMet) is the predominant methyl donor for biological methylations in important processes such as metabolism, gene regulation and ribosome assembly. The lack of a versatile chemical handle on the methyl group, however, hinders the use of methyltransferase enzymes as unique catalysts for selective chemical modification of biomolecules. This might be circumvented through the use of AdoMet analogues which might transfer unnatural functional groups, regioselectively, to the natural substrates (DNA, RNA, lipids for example) of these methyltransferases. However, previously studied AdoMet analogues have exhibited limited reactivity, which have been further compounded by the inherent instability of these sulphonium salts. In this study, a variety of AdoMet analogues lacking regions of the AdoMet structure that contribute to its instability were synthesized by direct chemoselective alkylation and their reactivity assessed using the enzyme thiopurine methyltransferase. Biochemical assays indicate comparable enzyme activity with three of the four analogues examined thus far. These results were subsequently confirmed by chemical analysis of the purified reaction products. These findings indicate that AdoMet analogues lacking regions of the parent molecule can serve as suitable methyltransferase substrates and can facilitate the transfer of unnatural groups to methyltransferase substrates.

152 18:30 Saturday CIBC Hall (MUSC)

Investigating Phosphonate in the Metagenome **M Taglione** <*mike.s.taglione@gmail.com*> and **G Horsman** <*ghorsman@wlu.ca*>, Wilfrid Laurier University.

Phosphonates (C-P compounds) are an underexplored class of bioactive natural products that are excellent targets for metagenomic discovery. Phosphonate compounds are present in microorganisms and show potential within the pharmaceutical and agricultural industries. However, few are known and their biosynthesisis is not well characterized. The biosynthetic entry point for most phosphonate compounds is phosphoenolpyruvatemutase (PEP mutase), which converts PEP to phosphonopyruvate (PnPy). Ten libraries acquired from the Canadian MetaMicroBiome Library (CM²BL) were screened using PCR for the PEP mutase enzyme. Hits were obtained in four libraries and clones were isolated from one library (Boreal Forest, 5BF) using serial dilution PCR. Isolated clones were sequenced and phosphonate production was examined by HPLC-DAD-ELSD. Sequencing revealed 84% amino acid identity with the PEP mutase gene product from the bacteria Burkholderia sp.CCGE1002, thereby confirming the presence of the enzyme within the isolated clones. The HPLC-DAD-ELSD analysis showed a new peak produced in clones compared to an empty vector control, but more needs to be done to analyze the compound present. Furthermore, the genes flanking PEP mutase in Burkholderia sp.CCGE1002 encode for AEP biosynthesis, suggesting the isolated clone may encode for AEP production. This study demonstrates the potential of a metagenomic platform for discovering phosphonates and their biochemical machinery.

153 18:30 Saturday CIBC Hall (MUSC)

Synthesis of Probes for the Activity-Based Profiling of Lipid Kinases **C. A. Cornacchia** <*Christina.Cornacchia@nrc-cnrc.gc.ca*>, **A. D. Hunt**, **A. Sherratt**, **S. O'Hara**, **C. S. McKay** and **J. P. Pezacki**, Life Sciences Division, Medical Devices Portfolio, National Research Council Canada.

Phosphoinositides are phosphorylated membrane phospholipids involved in numerous cellular processes including signal transduction and intracellular trafficking. Phosphorylation of these lipids results from lipid kinase activity; notably, misregulation of this class leads to a number of diseases, such as diabetes, cancer, and is even exploited by the hepatitis C virus (HCV)[1]. Lipid kinase activity, in turn, is regulated through effector protein interactions and post-translational modifications and may not directly correlate with protein abundance. As such, activity-based protein profiling (ABPP) can be used to assess target kinase activity in complex proteomic samples. ABPP uses active site-directed covalent probes to report on the functional state of enzymes.To determine changes in lipid kinase activity, several ABPP probes were synthesized based on the reversible kinase inhibitor, PIK93, due to its antiviral effects on HCV replication[2]. A benzophenone group capable of photo-crosslinking with proximal protein was introduced to convert PIK93 into a covalent ABPP probe. Additionally, a terminal alkyne handle was included in the probe so a reporter tag could be added via click chemistry. To achieve optimal labelling of lipid kinases, a study of several probes was performed, by modifying the linker lengths and functionality. A detailed overview of the synthesis, probe structure and preliminary labelling results of the PIK93-based probes will be discussed.

[1] Workman, P; et al. *Cancer Res*. **2010**, *70*, 2146.
[2] Miller, S; et al. *Science*. **2010**, *327*, 5973.

154 18:30 Saturday CIBC Hall (MUSC)

H477R PEPCK Alternates Ω loop Lid Domain Interaction Characterized Through Kinetic Studies **D Cui** and **T Holyoak**, University of Waterloo.

Phosphoenolpyruvate carboxykinase (PEPCK) is an enzyme functioning in the gluconeogenic pathway, and catalyzes the conversion of OAA to PEP. Based on previous structural and kinetic studies, it is recognized that the enzyme contains a 10-amino Ω loop domain that forms a mobile lid domain and this lid is an essential element required for enzyme function. The structural data demonstrate that the Ω loop occupies two distinct conformations, an open and closed conformation. The data also suggest that the closed-lid conformation becomes more energetically favourable as ligands interact with the enzyme. In the current work we sought to further explore the energetic coupling of ligand binding to the closure of the Ω loop lid by increasing the intermolecular interaction of the lid domain to the body of the enzyme and further stabilizing the closed lid conformation. To carry out this perturbation we introduced a point mutation (H477R) to the region of the enzyme body that interacts with the mobile Ω loop lid domain. Kinetic characterization of the mutated PEPCK enzyme demonstrates a decrease in catalytic activity as well as an increase in the apparent PEP substrate affinity. This data is consistent with the model that the H477R point mutation has caused a shift in the conformation equilibrium of the lid domain towards the closed state which decreases the catalytic function of PEPCK by preventing available substrates to bind to the active site or hindering the release of products.

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Structural and functional characterization of ClpP1-4 in acyldepsipeptide producing *Streptomyces hawaiiensis* **H Desai** <*desaihr@mcmaster.ca*>, **L Xing**, **P Patel**, **L Homchaudhuri**, **J Alexopoulos** and **J Ortega** <*ortegaj@mcmaster.ca*>, Department of Biochemistry and Biomedical Sciences & M. G. DeGroote Institute for Infectious Diseases Research,, McMaster University, , 1200 Main Street West, , Hamilton, ON L8N3Z5, Canada.

Caseinolytic protease (ClpP) is a serine protease that requires ATPases to degrade misfolded or damaged cellular proteins. ClpP is highly conserved across prokaryotes and eukaryotes. Recently, acyldepsipeptide antibiotics (ADEPs) have been shown to activate and disregulate ClpP. The compound ADEP is produced by *Streptomyces hawaiiensis* (Sh), which encodes six ClpP homologs, termed ClpPADEP and ClpP1- 5. Here we perform structural and functional characterization of these ShClpPs to elucidate the self-protection mechanism against ADEP adopted by *S. hawaiiensis*. ClpP1-4 were separately overexpressed in E. coli and purified using salting out, ion-exchange chromatography and size exclusion chromatography. To test whether the purified ShClpPs were catalytically active in vitro, we performed fluorimetric assays using different substrates. To access the oligmeric state for each ClpP, we used size-exclusion chromatography, dynamic light scattering and electron microscopy. The biochemical analysis showed that individually each ClpP lacked or had little peptidase activity. However, equimolar addition of ClpP1 and ClpP2 showed enhanced peptidase activity, suggesting a formation of active, mixed ClpP1P2 complex. Moreover, most ShClpPs appeared to form heptameric or tetradecameric ring like structures as observed through structural analysis. By investigating ShClpP activation by ADEP, the biological interactions of the ClpP-ATPase system can be further understood.

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A Biosensor: The Ability of a Histidine Peptide to Coordinate Metal Ions **Y Cao** <*yanshan.cao@mail.utoronto.ca*> and **H.-B. Kraatz** <*bernie.kraatz@utoronto.ca*>, Department of Physical and Environmental Sciences, University of Toronto Scarborough, 1265 Military Trail, Toronto, ON, M1C 1A4.

The ability to detect and monitor levels of metal ions is important in assessing the toxicity of various metal ions. Research on the possibility of using biosensors to detect metal ions rather than for traditional organic and biological molecules, are focus on more recently. Peptides are known to chelate effectively and specifically to a variety of metal ions through their amide nitrogen, carbonyl oxygen or the donor atom on their side chains. The imidazole group on the histidine has a very efficient nitrogen donor and can coordinate in a variety of ways depending on the position on the peptide chain.

A histidine peptide biosensor was made through immobilization of CDK2 peptide on a gold electrode modified with self assembled thiol monolayer (Figure 1). Its ability to bind metal ions was studied electrochemically using cyclic voltammetry and electrochemical impedancespectroscopy. The composition and the stiochiometry of the surface layer was confirmed by XPS and ESI-MS. The Histidine peptide was shown to bind to various metal ions.

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Evaluating the refolding interactions of hisactophilin, a myristoylated protein **M. Lemke** <*mflemke@uwaterloo.ca*>, **D. MacKenzie** <*d2macken@uwaterloo.ca*>, **M. Smith** <*martintjsmith@gmail.com*> and **E. Meiering** <*meiering@uwaterloo.ca*>, Guelph-Waterloo Centre for Graduate Work in Chemistry and Biochemistry, Deparment of Chemistry, University of Waterloo, 200 University Avenue West, Waterloo, Ontario, N2L 3G1.

Hisactophilin is an actin bundling protein that enables chemotaxis in Dictostelium discoideum. Hisactophilin displays the conserved β-trefoil structure, analogous to fibroblast growth factor and interleukin-1β. The N-terminal glycine of hisactophilin is covalently linked to a myristoyl group and exhibits a pH-dependent switching mechanism; at a pH higher than 6.95 the myristoyl group is sequestered within the core of the protein, and as the pH is lowered below 6.95 it can become accessible, allowing hisactophilin to reversibly interact with the plasma membrane. Myristoyl switches have been implicated in a number of signalling pathways, including recoverin of the retina. Mutants H90G and F6L were studied in both myristoylated and non-myristoylated forms to determine their interactions with the myristoyl group in the folding transition state. Histidine-90 lies within a β turn, and replacement of the histidine with a glycine is thought to increase flexibility and dynamics in this region. Phenylalanine-6 resides in the core of the protein and has been shown to interact with the myristoyl group; replacement of phenylalanine with leucine destabilizes hisactophilin. The refolding of H90G was studied using manual mixing and stopped flow techniques and was found to refold faster compared to wild type, suggesting stabilization of H90G over wild type. The destabilization of F6L has limited purification; refolding kinetics have not yet been determined.

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Heterologous Production and Characterization of hSRCR1 **M. Dorrington** <*dorrinmg@mcmaster.ca*>, **C. Yin**[a,c] <*yincy@mcmaster.ca*> and **D. Bowdish** <*bowdish@mcmaster.ca*>, [a]McMaster Immunology Research Centre, McMaster University, Hamilton, ON, L8S 4L8; **A. Huynh**[b,c] <*huynha8@mcmaster.ca*> and **A. Guarne** <*guarnea@mcmaster.ca*>, [b]Department of Biochemistry and Biomedical Sciences, McMaster University, Hamilton, ON, L8S 4L8; [c]Integrated Science, McMaster University, Hamilton, ON, L8S 4L8.

Since ancient times, organisms have used the innate immune system to protect themselves from invading pathogens. Macrophages help facilitate this function by recognizing, internalizing, and destroying harmful substances. Found on macrophages are scavenger receptors which have a broad binding specificity that is used to discriminate between self and non-self substances. One specific receptor, the macrophage receptor with collagenous region (MARCO), plays a critical role in protecting organisms against airborne pathogens. Like other receptors in the same class, it was believed to only bind polyanions, but it has been recently found that the SRCR domain of MARCO also binds bacterial ligands. However, no specific ligand has been identified. To search for possible MARCO-binding bacterial ligands, we have expressed and purified recombinant variants of MARCO containing the SRCR domain. Furthermore, these constructs have been shown to specifically bind to *Streptococcus pneumonia*, one of many nasopharynx infections known for causing meningitis, sepsis, and pneumonia. By having these constructs, further studies can be pursued to identify specific ligands, determine the structure of this region of MARCO, and define which region of MARCO binds to what type of ligand: polyanions vs. bacterial ligands. Our work sets the foundation to look for MARCO-binding bacterial ligands. Future work will include the structure determination of this fragment of MARCO bound to its bacterial ligands in order to elucidate how the interaction occurs at the

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Novel protein-based siRNA-delivery agents and their enhancement through promoting endosomal escape. **W. Wang**[a,b] <*wwang059@uottawa.ca*>, **D.C. Danielson** <*Dana.Danielson@nrc-cnrc.gc.ca*> and **J.P. Pezacki**[a,c,d] <*John.Pezacki@nrc-cnrc.gc.ca*>, [a]Department of Biochemistry, Microbiology & Immunology, University of Ottawa; **N. Sachrajda** <*natalie.sachrajda@rogers.com*>, Department of Biology, University of Ottawa; [b]Department of Chemical and Biological Engineering, University of Ottawa; [c]National Research Council of Canada, Life Sciences Division, 100 Sussex Drive; [d]Department of Chemistry, University of Ottawa.

RNA silencing is the highly conserved cellular process that allows targeted gene knockdown using exogenous short-interfering RNAs (siRNAs). siRNAs are widely pursued for human therapy since they have the potential to knock down expression of almost any disease-causing gene. A major hurdle in using siRNAs clinically is their inability to enter the cellular cytoplasm when added exogenously due to their large size and highly anionic charge. Therefore, there is widespread interest in developing siRNA delivery agents. Peptide transduction domains (PTDs) are small, highly cationic peptides that allow cell entry of attached cargo. In this study, we report a novel siRNA delivery agent based on the p19 protein, which is a siRNA-binding protein endogenous to tombusviruses. We have generated novel recombinant fusion proteins using a linked p19 dimer fused with the PTD, TAT, and applied them to cellular delivery of siRNAs in human hepatoma cells to induce gene knockdown. Furthermore, we improve the potency of gene knockdown by promoting endosomal escape of the p19:siRNA complex through co-incubating the treatment with a pH-dependent endosomolytic peptide 'E5' derived from the Influenza HA2 domain. We also present our progress in developing p19-2x-TAT fusion proteins that include this endosomolytic E5 domain.

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Optimising *Giardia lamblia* cytochrome b_5-l expression conditions in minimal media as a prelude to structural 2-D NMR spectroscopy **M.S. Mesbahuddin**, **S. Rafferty** and **J. Yee**, Trent University.

The water-borne protozoa *Giardia lamblia* encodes three members of the cytochrome b_5 family of unknown function. Major predicted differences between gCYTb_5-l and microsomal cytochrome b_5 (the most well-characterized family member) are i) a lower density of surface acidic residues about the exposed heme edge ii) the presence of more hydrophilic residues within the heme-pocket iii) the presence of unique N- and C-terminal extensions flanking the core heme-binding domain. I intend to use Nuclear Magnetic Resonance (NMR) spectroscopy to determine the structure of gCYTb_5 but first must optimize its expression in the minimal media required for isotope-labelled protein. By comparing gCYTb_5 levels from expression experiments with different vector backbones, temperature, carbon sources and induction conditions I found that expression was highest with a kanamycin resistant vector, 37C incubation, a glycerol carbon source and harvesting four hours after induction with both IPTG and the heme precursor 5-aminolevulinic acid.

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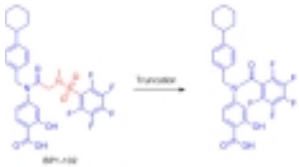
Synthesis of Truncated Stat3 Inhibitors for Anticancer Therapy **R. Colaguori** <*robert.colaguori@utoronto.ca*>, **B. D. G. Page** and **P.T. Gunning**, The Gunning Group, University of Toronto Mississauga, Mississauga, ON, L5L 1C6.



Signal transducer and activator of transcription 3 (Stat3) protein is a cytosolic transcription factor that is emerging as a promising target for anti-cancer development. Cancer cells often demonstrate aberrant Stat3 activity which has been identified as a driving force behind the development and progression of a number of cancers. Previous work from our lab has led to the development of some of the most potent Stat3 inhibitors in the literature. Current lead compound BP1-102 demonstrates potent anti-cancer activity against human breast and lung cancer mice xenografts at doses as low as 3 mg/kg[1]. Recent efforts from our research group aim to improve pharmacokinetic properties of BP1-102 by decreasing molecular weight, increasing membrane permeability, and improving metabolic stability. This presentation will highlight the design and synthesis of truncated BP1-102 derivatives that demonstrate potent activity against Stat3 and are hoped to play a key role in the fight against cancer.

[1] Zhang, Xiaolei; Yue, Peibin; Page, Brent D. G.; *et al*. Orally bioavailable small-molecule inhibitor of transcription factor Stat3 regresses human breast and lung cancer xenografts. *Proc. Natl. Acad. Sci.* **2012**, *109*, 9623-8.

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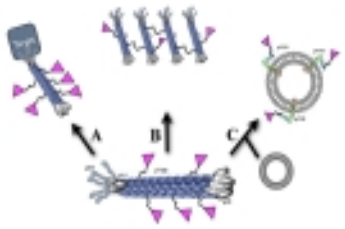
Investigating the use of bacteriophage M13 pVIII protein in biomaterials applications **C. Rowan** <*cjrowan@uwaterloo.ca*>, **A. Petrie**, **E. Daub** and **J.F. Honek** <*jhonek@uwaterloo.ca*>, Department of Chemistry, University of Waterloo.



Filamentous bacteriophage M13 is a lysogenic phage that infects *E. coli*. M13 is most commonly known for its applications in phage display and more recently, nanotechnology. The virus contains ~2700 copies of the outer coat protein pVIII, a small ∝-helical protein that surrounds the ssDNA genome. The pVIII protein consists of 73 amino acids (a.a.) with a N-terminal 23 amino acid leader peptide sequence that is cleaved yielding a 50 a.a. mature form that is incorporated into the virus. Mature pVIII has an outward facing N-terminal region and an inward facing C-terminus that interacts with the phage DNA.

We propose to use M13 as a novel flexible targeting platform by manipulating the amino acid sequence by introducing unnatural amino acids into pVIII. These pVIII proteins will be selectively modified using bioorthogonal chemistry to attach a variety of functional groups and biophysical labels to pVIII. Possible downstream applications of this modified pVIII include phage targeting systems (A), controlled crosslinking of M13 to produce novel nanofibres (B) and targeted liposomes (C).

INDEX of Authors

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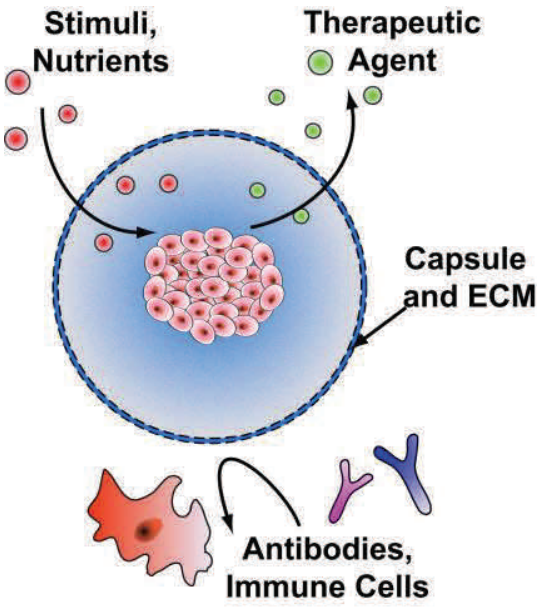

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