

**Schedule of Events**

November 4th-6th, 2016

Cairns Family Health and Bioscience Research Complex, Brock University

St. Catharines, ON

**Friday, November 4th**

4:00 pm-5:00 pm **Registration** (Cairns Complex Scotiabank Atrium)

 **Brock Graduate Studies Information Session**

5:00 pm-8:00 pm **Welcome Mixer**

**Saturday, November 5th**

9:00 am - 9:30 am **Registration** (Welch Hall, Room 324)

9:30 am - 9:40 am **Introductory Remarks**

9:40 am - 11:00 am **Oral Presentations**

11:00 am - 11:30 am **Coffee Break**

11:30 am- 12:00 pm **Oral Presentations**

12:10 pm - 1:30 pm **Lunch** (Cairns Complex, 5th floor)

 **Poster Set-Up**

1:40 pm - 3:00 pm **Oral Presentations** (Welch Hall, Room 324)

3:00 pm-3:10 pm **Break**

3:10 pm-4:50 pm **Oral Presentations with Keynote Address**

5:00 pm - 6:00 pm **Poster Presentations** (Cairns Complex, 5th floor)

7:00 pm **Dinner** (La Scala Ristorante, St. Catharines)

**Sunday, November 6th**

9:30 am- 12:10 am **Oral Presentations** (Cairns, Room 550)

12:10 pm-12:30 pm **Symposium Awards and Closing Remarks**

**Thank you to our sponsors and participants!**

**Oral Presentations**

**Saturday, November 5th**

Time: 9:30 am-12:10 pm (Welch Hall, Room 324)

**Opening Remarks**

9:30 am **Professor Travis Dudding, PhD** Brock University

**Presentations**

**Morning Session**

9:40 am **Farukh Iftakhar Ali** University of Guelph

Solid-State Green Synthesis of Diketopiperazines (DKPs)

10:20 am **Professor Andrew Murkin , PhD** University at Buffalo, SUNY

Mechanism of Enzyme-Catalyzed Retro-aldol Reactions in *Mycobacterium tuberculosis*

**Coffee Break**

11:30 am **Sneha Ray** University at Buffalo, SUNY

Propionate-3-nitronate is a covalent, reversible *Mt*ICL inhibitor

**Lunch**

**Afternoon Session**

1:40 pm **Philippe Archambualt** Concordia University

Exploring Weak Interactions in the GAAA Oligonucleotide Tetraloop

2:20 pm **Roya Mir, PhD** Brock University

Cyclopropeniums as a Platform for Catalysis

**Break**

3:10 pm **Professor J. Peter Guthrie, PhD** University of Western Ontario

Equilibrium Constants for Imine Formation by Computation Alone

**Keynote Address**

3:50 pm **Professor Mark Taylor, PhD** University of Toronto

Physical Organic Chemistry in Molecular Recognition and Catalysis

**Sunday, November 6th**

Time: 9:00 am-12:30 pm (Cairns Complex, Room 550)

**Presentations**

**Morning Session**

9:30 am **Antoine Juneau** Université du Québec à Montréal

Mechanistic Insights in Iridium/Nickel Co-Catalyzed Photoredox Cross-Coupling Reactions

10:10 am **Professor S. Holger Eichhorn, PhD** University of Windsor

Synthesis and Interfacial Properties of an Amphiphilic Tetraazaporphyrin

10:50 am **Professor Dmitriy V. Soldatov, PhD** University of Guelph

Pyrolysis of Short Linear Peptides in the Solid State and Gaseous Phase

11:30 am  **Professor Olivier Lebel, PhD** Royal Military College of Canada

Mexylaminotriazines: an Efficient and Modular Approach for the Design and Synthesis of Glass-Forming Materials for Organic Photonics

**Closing Remarks**

12:10 pm **Professor Travis Dudding, PhD** Brock University

**Poster Presentations**

Time: 5:00 pm- 6:00 pm (Cairns Complex, 5th Floor)

**Poster 1. Janet Gaba** and Heidi Muchall\*

*Department of Chemistry, Concordia University, Montreal, QC*

# Computational Study Into the Origin of Chemical Shift Changes Upon Formation of Weak Interactions

**Poster 2. Richard Le Sueur**, Lee Belding, Peter Stoyanov, and Travis Dudding\*

*Department of Chemistry, Brock University, St. Catharines, ON*

Development of a Class of Cyclopropenimine-Based Proton Sponges

**Poster 3.**  **Roya Mir**, Ivor Smajlagic, Rozhin Rowshanpour and Travis Dudding\*

 *Department of Chemistry, Brock University, St. Catharines, ON*

Phase-Transfer Catalyzed O-Silyl Ether Deprotection Mediated Cyclopropenium Cation

**Poster 4. Katie Dempsey** and Travis Dudding\*

 *Department of Chemistry, Brock University, St. Catharines, ON*

Synthesis of Cyclopropenimine-Functionalized Ylidene-Triazenes

**Poster 5. Anthony Antoniani**, Vanessa M. Bellemore, Matt Halloran, Ed Cieplechowicz and Kenneth Maly\*

*Department of Chemistry and Biochemistry, Wilfrid Laurier University, Waterloo, ON*

Self Assembly of hexaalkoxydibenzo[a,c]pentacenequinones

**Poster 6. Sahar Nikoo** and James W. Gauld\*

*Department of Chemistry and Biochemistry, University of Windsor, Windsor, ON*

Computational Studies on the Reactivity of C-Terminal Cysteines with HNO

**Poster 7.** Yi Pan and **Mónica Barra**\*

*Department of Chemistry, University of Waterloo, Waterloo, ON*

Computational study of solvent hydrogen-bonding effect on the barrier to isomerization of phenyltriazenes

**Poster 8. Aaron J Smith**, Farukh I Ali, Dmitriy V Soldatov\*

 *Department of Chemistry, University of Guelph, Guelph, ON*

Thermally-Induced Transformations in Short Chain Homopeptides: Leucine vs Glycine

**Poster 9. Patrick L. Fernandez** and Andrew S. Murkin\*

Department of Chemistry, University at Buffalo, SUNY, Buffalo, New York, United States

The Transition State of D-Alanine:D-Alanine Ligase as a Potential Drug Target for Treatment of Tuberculosis

**Poster 10. Nicole LeGrow** and Kenneth E. Maly\*

 *Department of Chemistry and Biochemistry, Wilfrid Laurier*

 *University, Waterloo, Ontario, N2L 3C5, kmaly@wlu.ca*

Synthesis and Characterization of Hydrogen Bonding Liquid Crystals