



47th Ontario-Quebec Physical-Organic Minisymposium

York University | Nov 1-3, 2019

# Welcome to POMS-47 at York!

After a long hiatus, we are excited to host the 47<sup>th</sup> annual Ontario-Quebec Physical Organic Minisymposium (POMS) again at York University.

And it is timely to do so. York has been undergoing an impressive transformation and modernization in recent years with considerable growth, particularly in the areas of Science and Engineering that are supported by several new, state-of-the-art buildings. Moreover, the opening of two new subway stations on campus now conveniently connects York to downtown Toronto. Walk around campus and see for yourself.

As you know, POMS is one of North America's premier physical organic chemistry symposia. The meeting showcases all aspects of physical organic chemistry and its relentless, evidence-based approach to understand chemical processes: from fundamental mechanistic investigations and spectroscopy to advanced materials and biological chemistry. All fields of chemical science can benefit from the foundational principles of physical organic chemistry, and POMS is a great place to see these principles in action. Moreover, POMS has always been a venue that embraces the next generation of scientists – and this year makes no difference. We are delighted to have many students and postdocs present their research again in a stimulating, friendly, and inclusive environment.

Thank you for joining us for an exciting symposium.

Thomas Baumgartner & Chris Caputo

# POMS-47 would not be possible without the help of the following generous sponsors:













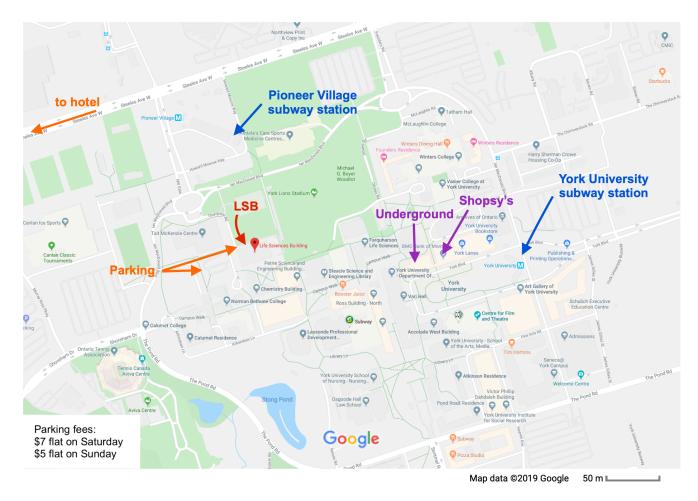


# **POMS Locations**

All scientific sessions take place in the Life Sciences Building (LSB, shown on the cover). All lectures are in room LSB 103, and registration, poster sessions, and breaks are in the foyer outside the lecture room. The main entrance to LSB is on the west side.

Opening Mixer (Friday 7-9 pm): Join us for drinks at The Underground – in the basement of the old Student Centre, next to Vari Hall.

Conference Dinner (Saturday 7-10 pm): Shopsy's – inside York Lanes (registration required).



An interactive campus map can be accessed here:

https://map.concept3d.com/?id=1200#!s/?ct/29101,29093

# Registration

On-site registration is available on Friday evening at the Opening Mixer in the Underground, or Saturday morning in LSB, starting at 8:30 am.

# **Instructions for presenters**

# **Talks**

The lecture room is equipped with a PC-system running the latest versions of Microsoft Office, and Acrobat Reader. You are also free to bring your own laptop, if you wish. The media system has VGA and HDMI connectors (don't forget to bring your own adaptor). Please provide your files and/or check your connections before the start of your session.

The allotted time for your presentation is 15 minutes + 5 minutes for discussion.

# **Posters**

The size of the poster boards allows for standard sized (3'x4') posters in either portrait or landscape orientation. Push pins will be provided. Please mount your posters during the lunch break and take them down again after the poster session on Saturday evening.

# Internet access

YorkU is a member of the eduroam wireless network.

In addition, YU provides wireless guest access through AirYorkGUEST.

# **Final Schedule**

All scientific events will take place in the Life Sciences Building (LSB) on YorkU's Keele campus

# Saturday, November 2

• *		
8:55 - 9:00 am	Welcome & Introduction	LSB 103
9:00 - 9:20 am	Daniela Cappello	01
9:20 - 9:40 am	Ivor Smajlagic	02
9:40 - 10:00 am	Simanga Gama	О3
10:00 - 10:30 am	Coffee Break (refreshments provided)	
10:30 - 10:50 am	Sami Sabbah	04
10:50 - 11:10 am	Monika Snowdon	О5
11:10 - 11:30 am	Robert Pollice	<b>O</b> 6
11:30 - 11:50 am	Nicholas Dogantzis	07
11:50 am - 12:10 pm	Justin Kai-Chi Lau	08
12:10 - 12:30 pm	Audithya Nyayachavadi	О9
12:30 - 2:00 pm	Lunch (provided)	
2:00 - 2:20 pm	Ehsan Hosseininassab	O10
2:20 - 2:40 pm	Gabriel dos Passos Gomes	011
2:40 - 3:00 pm	Michael Ocheje	012
3:00 - 3:20 pm	Janet Gaba	013
3:20 - 3:40 pm	Break	
3:40 - 4:00 pm	Joshua Gaffen	014
4:00 - 4:20 pm	Bhupinder Metneja	015
4:20 - 4:40 pm	Zainab Shakeel	016
4:40 - 5:00 pm	Daliane Regis Correa da Silva	017
5:00 - 6:30 pm	Posters (refreshments provided)	LSB lobby
6:30 - 6:45 pm	Student Award Presentations	•
7:00 - 10:00 pm	Conference dinner (registration required)	Shopsy's
	, O	1 - 7 -

# Sunday, November 3

		LSB 103
9:00 - 9:20 am	Ryan Hili	018
9:20 - 9:40 am	Ken Maly	019
9:40 - 10:00 am	Ron Kluger	O20
10:00 - 10:30 am	Coffee Break (refreshments provided)	
10:30 - 10:50 am	Kjell Jorner	021
10:50 - 11:10 am	Jean Bouffard	022
11:10 - 11:30 am	Will Skene	023
11:30 - 11:50 am	Mathieu Frenette	024
11:50 am - 12:10 pm	Holger Eichhorn	O25
12:10 - 12:20 pm	Closing	

# **List of Talks**

# Saturday, Nov. 3

# O1 Daniela Capello, University of Western Ontario

"Exploring the Optoelectronic Properties of Double-Rotor Boron Difluoride Hydrazone Dyes"

## O2 Ivor Smajlagic, Brock University

"Mechanistic Insight Towards Understanding The Role Of Charge In Thiourea Organocatalysis"

# O3 Simanga Gama, Queen's University

"PhnY\*/PhnZ-Catalyzed Oxidative Cleavage of the C-P Bond in Organophosphonates"

## **O4 Sami Sabbah**, Université du Québec à Montréal

"Looking for Cationic Phenol: A Mechanistic Study of De-Aromatization Reactions Induced by Hypervalent Iodine"

#### **O5** Monika Snowdon, University of Waterloo

"Advancements in the alignment relay technique of single walled carbon nanotubes using a carboxylic acid moiety"

#### O6 Robert Pollice. ETH Zürich

"A Universal Quantitative Descriptor of the Dispersion Interaction Potential"

## O7 Nicholas Dogantzis, Ryerson University

"Optical Patterning with Photoactivated and Nanoparticle-Enhanced Fluorescence"

#### **O8 Justin Kai-Chi Lau**, York University

"Loss of Water from Oligopeptides and their [bn]+ ions"

# **O9 Audithya Nyayachavadi**, *University of Windsor*

"Crosslinking of Conjugated Polymers with Polydiacetylenes: A New Approach for Processing and Patterning Organic Semiconductors"

# **O10 Ehsan Hosseininassab**, *Université du Québec à Montréal*

"Investigating the Secondary Autoxidation of Hydroperoxides via  $\alpha C$ -H Abstraction to Generate Hydroxyl Radicals: Fluorene Autoxidation as a Model System"

#### O11 Gabriel dos Passos Gomes. University of Toronto

"Machine Learning Reactivity in the Chemical Space of the Vaska's Complex"

# O12 Michael Ocheje, University of Windsor

"Stretchable and Healable Conjugated Polymers Towards Electronic Materials with Biomimetic Properties"

## O13 Janet Gaba, Concordia University

" $\pi$ - $\pi$  stacking as a driving force in film formation at the air-water interface"

#### O14 Joshua Gaffen, York University

"Fluorescent Lewis Acid/Base Adducts (FLA): A Simple Method for Determining Lewis Acid Strength"

## O15 Bhupinder Metneja, Concordia University

"An Algorithm to Explore Molecular Potential Energy Surfaces based on the Activation-Relaxation Technique"

# O16 Zainab Shakeel, Ryerson University

"Silyloxy Porphyrin Silanes: Tunable 3-dmensional photo- and electroactive compounds"

## O17 Daliane Regis Correa da Silva, University of Ottawa

"Development of Metal Oxide Nanofibers as potential antimicrobial agents"

# Sunday Nov. 3

## O18 Ryan Hili, York University

"Chemical tools to sequence DNA and RNA methylomes"

# O19 Ken Maly, Wilfrid Laurier University

"Novel Heterocyclic Acene Derivatives: Synthesis and Self-Assembly"

# **O20** Ron Kluger, University of Toronto

"Differences in Protonation vs Elimination from Related Carbanions as Reaction Clocks"

# **O21 Kjell Jorner**, Astra Zeneca

"Combining physical organic chemistry and machine learning for reaction prediction to guide route selection and design"

#### **O22 Jean Bouffard**, Ewha Womans University (Seoul)

"Less Conventional Applications of Persistent Carbenes in Organic Materials Chemistry and Catalytic Synthetic Methodology"

## **O23 Will Skene**, Université de Montréal

"How to Improve Color Retention in Electrochromic Devices"

# **O24** Mathieu Frenette, Université du Québec à Montréal

"Mechanistic Insights and Innovative Solutions in (Photo)Redox Catalysis"

## **O25 S. Holger Eichhorn**, *University of Windsor*

"Side-Chain Free Donor-Acceptor Dyes Prepared By Sequential Substitution of Cyanuric Chloride"

# **List of Posters**

# P1 Aviya Akari, Ryerson University

"Photochemical Free-Radical Processes for Lithographic Applications"

## P2 Abdel Al Ahmad, Université de Montréal

"Component exchange for multiple property tailoring"

## P3 Michael Anghel, University of Western Ontario

"Synthesis and Characterization of a Nitronyl Nitroxide Radical Polymer"

# P4 Nayanthara Asok, York University

"An Unexpected "Step-Conjugated" Biphosphole via Unique P-P Bond Formation"

## **P5** Monica Barra, University of Waterloo

"Kinetic Study on the Thermal Z-E Isomerization of Photoswitchable N-Acylhydrazones"

#### **P6 Jordan Bentley**, York University

"A Simple Method of Determining Lewis Acidity Using Fluorescence"

# P7 Michael Berteau-Rainville, Concordia University

"Computational Insight into Affinities of Boranes to Sulfur- and Nitrogen-Containing Organic Semiconductors"

# **P8** Asma Boushih, Université du Québec à Montréal

"Inexpensive Label to Report a Critical Temperature Breach and Duration via Sequential Colour Changes"

## **P9** Francis L. Buguis, University of Western Ontario

"Synthesis and Characterization of Amine-Substituted Boron Difluoride Formazanate Dyes"

## P10 Brenden Carlson, Brock University

"Charge-Enhanced Thioureas as Hydrogen Bond Donors for Friedel-Crafts Alkylations"

# **P11 Judith Cristobal**, State University of New York at Buffalo

"Glycerol 3-Phosphate Dehydrogenase: Interactions between Substrate and Activators with K120, R269 and Q295 Side Chains"

# P12 Michael Denk, University of Guelph

"Nature's Hydrides: CBS-QB3, CCSD(T), and Double Hybrid Thermochemical Calculations"

#### **P13** Jasveer Dhindsa, University of Western Ontario

"Optoelectronic Properties of a Polymer and Model Complexes Derived from Boron Difluoride Formazanate and Platinum(II) Diynes"

## **P14** Kelsey Fournier, University of Ottawa

"Porphyrin-decorated Glass Wool for Water Remediation"

## P15 Karol Golian, Ryerson University

"Fluorescence Mapping of Nanoscaled Plasmonic Fields"

#### P16 Masoud Harati, University of Windsor

"Polymerization of Globular Hexaphenyloxycyclotriphosphazene Derivatives Containing Diacetylene Groups"

#### **P17** Trevor Harris, University of Pennsylvania

"Sterics and Stereoelectronics in Aza-Glycine: Impact of Aza-Glycine Preorganization and H-bonding in Collagen Peptides"

# P18 Lana Hiscock, Wilfrid Laurier University

"Controlling  $\pi$ -Stacking Interactions in a Series of Novel Heteroacene Derivatives"

# **P19** Taylor Hope, Université du Québec à Montréal

"Mechanistic Insight into Fe Catalyzed (alpha)-C-H Oxidations of Tertiary Amines: Non-Radical Pathways for Base-Metal Catalyst"

## **P20** Graeme Howe, Queen's University

"Temperature-Independent Kinetic Isotope Effects as Evidence for Extensive Hydride Tunneling in Phosphite Dehydrogenase"

#### **P21** Benjamin Katzman, University of Western Ontario

"Synthesis & Characterization of Nucleobase-Containing Boron Difluoride Formazanate Complexes"

## P22 Amrita Kaushik, Noida Institute of Engineering and Technology

"Data Validation by FIS for Heavy Metal Ions Removal Using Husk of Cajanus Cajan in Aqueous Solution"

## **P23 Josh LeDrew**, Wilfrid Laurier University

"Synthesis and Self-Assembly of Liquid Crystalline Triphenylenedicarboxythioimides"

# **P24** Michael Lerond, Polytechnique Montréal

"Towards organic stretchable conductive films"

#### **P25** Stephanie Lo, York University

"Viologen-based Polymers for Organic Batteries"

## **P26** Gage Mason, University of Windsor

"Photophysical and Optical Properties of Semiconducting Polymer Nanoparticles Prepared from Hyaluronic Acid and Polysorbate 80"

## **P27** Madison Mooney, University of Windsor

"Development of Degradable and Water-Soluble Semiconducting Polymers for Greener Printed Electronics"

# **P28** Eric Nicol, University of Guelph

"A Computational Investigation of a Triaryl Oxathiin Synthesis and Base Induced Decomposition"

#### **P29** Julia Pignanelli, University of Windsor

"Investigating the Self-Healing Efficiency in Soft Polymers Through Dynamic Metal-Ligand Interactions"

# P30 Mehdi Rezapour, University of Windsor

"Topochemical Polymerization of 1,3-Butadiyne in the Gel State Toward New Electroactive Polymers"

## **P31** Adam Riddell, University of Guelph

"Exploring the Synthesis of Allenyl Sulfoxides from Thioimides"

# **P32** Rozhin Rowshanpour, Brock University

"Selective Aerobic Oxidation of Benzylic Alcohols Catalyzed by a Dicyclopropenylidene-Ag(I) Complex"

#### **P33** Scott Sammons, University of Guelph

"Diastereoselective Alkylations of N-Protected-Beta-Aminosulfenate Anions"

## P34 Farsheed Shahbazi Raz, University of Windsor

"Computational study and synthesis of a novel dual-targeting probe for prostate cancer molecular imaging"

# P35 Lénaïc Soullard, University of Windsor

"Investigation of the Mechanical Properties of Organic Semiconductors by Soft Lamination Techniques"

## P36 Sahana Sritharan, Ryerson University

"Exploring BODIPY-phenylacetylene rotaxanes as artificial photosynthetic systems"

## **P37** Blake St. Onge, University of Windsor

"Investigation of Metal-Ligand Interactions and their Effect on Electronic Properties in Semiconducting  $\pi$ -Conjugated Polymers"

# P38 Seyedeh Maryamdokht Taimoory, University of Windsor

"Novel axle scaffolds form high affinity interactions with crown ethers for the construction of cylindrical skeletons"

# P39 Seyedeh Maryamdokht Taimoory, University of Windsor

"Synergistic Application of Synthetic, Kinetic and Computational Methods to Study Host-Guest Chemistry, Graphene Based Surface Chemistry, Peptides, and Self-Immolative Polymers"

# **P40** Lavinia Trifoi, Ryerson University

"A Reconfigurable, Dual-Output Molecular Logic Gate"

# P41 Chengzhang Yao, Université de Montréal

"Dual Electrochromic and Electrofluorochromic Role of a Red Emissive Fluorophore"

## P42 M'hamed Chahma, Laurentian University

"Polythiophene radicals: Synthesis and Characterization"

## P43 Subashi Ubayawardhana, SUNY Buffalo

"Mechanistic Investigation of the Reaction Catalyzed by 5-methylthioribose 1-phosphate Isomerase in the Methionine Salvage Pathway"