

## **SOUSCC45 Technical Program**

8:30 - 9:30 - Sciex Breakfast, LAS Lobby

9:30 - 10:15 - Keynote, Dr. Voislav Blagojevic

10:30 - Sessions Start

### **Analytical**

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#### **Analytical I**

Alicia Mell	<b>Paul Piunno, Shaolong Zhu, CB122, 10:30 - 11:50</b> Risk Assessment of Smoke Exposure of Firefighters in the 2016 Fort McMurray Wildfire using GC-MS
Qusai Hassan	Lipid Signal Suppression for NMR-based Environmental Metabolomics In Vivo
Lisa Szymkowicz	Phospholipid-based model membrane system for hydrogen-deuterium exchange mass spectrometry of membrane proteins
Keuna Jeon	Optimizing Metallic Nanoplates for Plasmon-Enhanced Spectroscopies.

#### **Analytical II**

Tianxiao Ma	<b>Derek Jackson, Kerene Brown, CB129, 10:30 - 12:10</b> Investigation of Building and Testing Electrochemical Toll-like Receptor Sensor
Santiago Giron	An Environmentally Responsive Nucleoside Analog for Observing DNA Aptamer-Protein Interactions
Christian Ieritano	Characterization of a Wasp Venom Component with Selective Anticancer Activity via Gas-Phase Microsolvation with Differential Mobility Spectrometry
Trina Dang	The New Aldetective: Using CEST-MRI to Detect Endogenous Biological Aldehydes
Lisa Labine	Analysis of Tramadol and Metabolites in Skeletal Remains by UPLC-qToF MS: Effects of the Dose-Death Interval on Drug and Metabolite Levels

#### **Analytical III**

Natan Veinberg	<b>Paul Piunno, Shaolong Zhu, CB122, 1:40 - 3:00</b> A Solid-State NMR Study of Hydrated Active Pharmaceutical Ingredients
Martin Badley	Development of Quantitative X-ray Photoelectron Spectroscopy (XPS) Imaging
Yousef Risha	Development and validation of a LC-MS/MS method for quantitative analysis of Vancomycin in Canadian waste water treatment plants' effluent
Xia Zhu	Characterization of CO/CO <sub>2</sub> of emissions from on-road vehicles in the Greater Toronto Area

#### **Analytical IV**

Aiyun Yang	<b>Derek Jackson, Kerene Brown, CB129, 1:40 - 3:00</b> In-Situ High-Pressure Study of ZIF-67 and CO <sub>2</sub> Storage via Infrared Spectroscopy
Hamna Fayyaz	Silica Coated Magnetic Bead Extraction of DNA in a Microfluidic Device: A Module for a Lab-on-a-Chip Device for Rapid Species Identification
Jonathan Adsetts	Proton Transportation Across Ionic Liquid-Soaked Nafion Investigated by Scanning Electrochemical Microscopy
Heather Schwartz-Narbonne	Cleaning up our act: The heterogeneous reaction of gaseous bleach by-products with squalene as a surrogate for skin oil

#### **Analytical V**

William Zizek	<b>Paul Piunno, Shaolong Zhu, CB122, 3:30 - 5:10</b> Comprehensive Metabolomic Analysis of Serum from Peanut Allergic Children
Tianyi Wu	Time-resolved fluorescence of a binary dye mixture system: how well can lifetimes and amplitudes of be determined in selected-ion fluorescence experiments
Maria Karcz	Digital Microfluidic Platform for the Detection of Malaria Infection for Point-of-Care Applications
Yardley Cuthbert	Characterizing Hydroxyl-Substituted Polycyclic Aromatic Hydrocarbons
Iden Djavani-Tabrizi	Unimolecular Dissociation Reactions of Amino-Substituted PAHs using Collision-Induced Dissociation Mass Spectrometry (CID-MS) and RRKM Theory

### **Biological / Medicinal**

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#### **Biol / Med I**

Michaela Fernandes	<b>Bulent Mutus, Irina Oganessian, CB121, 10:30 - 11:50</b> Structure Activity Relationship (SAR) Study of a PAR4 Peptide Agonist
Rhys Powers	Involvement of B-/Z-DNA transition in the genetic flow of information
Yen Janette	Bioorthogonal click chemistry in the development of molecular imaging using aptamers
Jeremt Pak Hei	Helicobacter pylori NikR Mutant Characterizations for 19F NMR Structural Analysis

#### **Biol / Med II**

Amanda Tajik	<b>Gerald Audette, Ruth Knox, CB115, 10:30 - 11:50</b> Analysis of a stable bifunctional linker (N-methyl-O-(propyl-3-thiol) hydroxylamine) for carbohydrate-protein conjugation in vaccine development
Yanrui Zhu	Determining the thermodynamic binding characteristics of a ATP-binding DNA aptamer with ATP and other ATP analogues
Yun Jun Hho	Study of Slr1p in Schizosaccharomyces pombe lacking protein kinase
Richard Pulgarin	Conformational Dynamics of Glutathione S-Transferase on Benzo[a]pyrene Diol Epoxide via Hydrogen Deuterium Exchange Mass Spectrometry

**Bio/Med III**  
Emily Boehmer The intracellular localization of three isolates of cytochrome b5 during encystation of Giardia intestinalis  
Alexander Eddenden Synthesis of glycan constructs on polypeptides by a site-specific chemoenzymatic method using bacterial glycosyltransferases  
Alexa DiCecco Examining Allosteric of S-Nitrosoglutathione Reductase through Mutation of the First Twenty Amino Acids  
Mitchell DiPasquale Determination of the Role of CXXC Motifs in Cystathionine –  $\delta$ , – Lyase

**Bio/Med IV**  
Xiaojing Huang Characterizing lipocalin 2 conformational changes upon siderophore and iron binding using mass spectrometry  
Eliza McColl Probing the Heme Active Site of the Flavohemoglobin Enzyme in Giardia intestinalis  
Nadia Sharma Structural Characterization of Bioapatite in Mice Carrying the I130T Mutation of Connexin43  
Alexander Dewar Changes in flavohemoglobin expression on exposure of Giardia intestinalis to nitrosative stress

**Bio/Med V**  
Nicholas Bragagnolo Characterizing the Activity of a Novel Antiviral Protein Isoform from Phytolacca americana  
Caitlyn Bourque Cystathionine-gamma lyase/H2S system protects against LPS-induced inflammation in endothelial cells.  
Zeenat Ladak Anti-cancer drug resistance: Extrusion of anti-cancer drugs by multidrug resistant ABC transporters  
Jesse Ropat Selective Targeting of Cancer Cells by Exploiting Oxidative Stress Vulnerabilities with Novel Synthetic Curcumin Analogues

**Bio/Med VI**  
Carmen Kiltz Formation of nanoscale zero-valent iron (nZVI) using common weeds for the degradation of trichloroethylene  
Frank betancourt Identification of acyl-homoserine lactones and quantification of C-DI-GMP in pseudomonas fluorescens  
Nicholas Hodkinson Development of a High-Throughput Assay to Identify Novel [NiFe]-Hydrogenase Maturation Proteins in Escherichia coli  
Ian Fernandes Characterization of a Prediction Bifunctional Protein from Treponema denticola

**Bio/Med VII**  
Emily Tran Determining the structure of a putative  $\beta$ -helix motif of the Toc159 M-domain  
Margot Treidlinger Phospho-ubiquitin variants increase auto-ubiquitination activity of parkin E3 ligase  
Daniel Levin Creation of Microfluidic Devices for the Characterization of Macrophage Adhesion to Structured Silicon Dioxide Surfaces  
Jacob Pierscianowski Application of Oxime-Based Inhibitors of C-O Bond Cleaving  $\alpha$ -Carboxyketose Synthases as Neutral Phosphate Group Mimics in P-O Bond Cleaving Phosphatase

## Computational

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**Computational I**  
Roman Korol Tunneling to Hopping Crossover in Thermopower of the DNA Molecular Junctions  
Devan Kernaghan Predicting Partition Coefficients of Metallic Species Using COSMO-RS Solvation Theory  
Angela M. Murcia Rios Investigating the Rotary Mechanism of ATP Synthase Using Molecular Dynamics Simulations  
Johnny Luo Computational Insights into the Amino Acid Activation by Class I TrpRS and GluRS and Class II AspRS

**Computational II**  
Rachel McCormack A Computational determination of clustering in water vapour in the presence of charged species  
Bonnie Diep Quantum effects in the dynamics of sugars  
Chloe Clark Quantitative Structure-Property Modelling of Blood-Brain Barrier Partitioning  
Deborah Chan Farming Photons: Computational and Spectroscopic Studies of Phthalocyanines as a Photosensitizer in Dye-Sensitized Solar Cells

**Computational III**  
Tatiana Gatsak A model for orthohydrogen clusters  
Mark Zanon Developing Periodic, Localized Molecular Orbitals  
Jesse Vanloon Clustering by Self Organizing Maps of Conformations for Flexible Protein Domains obtained through Molecular Dynamics Simulations  
Tori Lambe Exploration of Conformational Isomerism of the Antibody SPE7 Using Molecular Dynamics Simulations

## Inorganic / Inorg. Materials

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**Inorganic I**  
Nadia Stephaniuk Inclusion Chemistry of Thiazyl and Selenazyl Radicals in MIL-53(Al)  
Jasveer Dhindsa Synthesis and Characterization of Push-Pull Polystannanes  
Jeanette Adjei Synthesis & Characterization of Oxazoline Ligands Containing Electron Donating Or Electron Withdrawing  
Daniel Cutler Exploring the Coordination Chemistry of ppmH as a New Ligand in 3d-Cluster Chemistry

**Inorganic II**

Scott Timmermans  
Daniela Cappello  
Erika Crowley  
Sarah Dale

**Chris Kerr, Jim Greene, LSB 107, 10:30 - 11:50**

Intramolecular Energy Transfer in Boron Difluoride 3-Cyanoformazanate Complexes  
Phosphonium Block Copolymers with Chiral Anions  
Glutaraldehyde Cross-linked Enzyme Aggregates Encapsulated in Ordered Mesoporous Silica  
Synthesis and coordination chemistry of a new arylazo ligand: Toward multifunctional spin-crossover materials

**Inorganic III**

Devon E. Chapple  
Alec Sherman  
Menandro Cruz  
Isaac De Vlugt

**Stephen Loeb, Louise Dawe, LSB101, 1:40 - 3:00**

Metal-Ligand Cooperative Catalysis for the Cyclization of Nitrogen Heterocycles  
Towards the Development of Cyclopropane Functionalized Gold Nanoparticles for Cycloaddition to Nitrone-Modified Substrates  
Investigation of the Dissolution and Self-Assembly of Polyferrocenyldimethylsilane Block Copolymer Micelles  
Infrared-Driven Charge Transfer in Transition Metal B12H12 Clusters

**Inorganic IV**

Maissa Belcina  
Rachel Langford  
Muntaser Farooq  
Samantha R. Anderson

**Jennifer Chen, Jim Greene, LSB 107, 1:40 - 3:00**

The Influence of a Donor on the Addition of Acrylonitrile to a Disilene  
1,2,3-dithiazolyl-o-naphthoquinone ligands for the development of switchable magnetic materials  
Cobalt (II/III) Oxazoline Complexes for Electrolyte Applications in Dye Sensitized Solar Cells  
The Role of Molybdenum in Corrosion Resistant Ni-Cr-Mo Alloys Exposed to Simulated Crevice Environments

**Inorganic V**

Scott Laengert  
Greg Yousif  
Vanessa T. Y. Lee

**Stephen Loeb, Louise Dawe, LSB101, 3:30 - 4:30**

Sequential Functionalization of a Natural Cross-linker Leads to Designer Silicone Networks  
The synthesis of acetal-free TF antigens, TACA disaccharides containing no labile glycosidic linkages  
Synthesis and Acidity Predictions of Unsymmetric Tripodal NPP'2 Iron Hydride Complexes

**Inorganic VI**

Doneique Menzies  
Declan DeJordy  
Kelly Wright

**Jennifer Chen, Jim Greene, LSB107, 3:30 - 4:30**

DNA Functionalization of Gold-Coated Silver Nanoprisms  
Design of new molecular magnetic materials utilizing 4-benzimidazole-1,2,3,5-dithiadiazolyl paramagnetic ligands  
Graphene Synthesis from Graphitic Sources by Ultrasonic Liquid Phase Exfoliation

**Organic / Org. Materials****Organic I**

Joseph Bedard  
Carling Renwick  
Vivekkumar Patel  
Robert Nanni

**Shegufa Mervchant, Andrei Nikolev, LSB103, 10:30 - 11:50**

Synthesizing and Engineering Next Generation Immobilized Antimicrobial Coatings  
New Hydrogen Bonding Modes of Activation of Donor-Acceptor Cyclopropanes  
Design, characterization and digestion of oil-in-water emulsions stabilized with Pickering fat crystals  
Synthesis and Reactivity of Gallium(I)-Crown Ether Compounds

**Organic II**

Cody Gale  
Rajeshwar Vasdev  
Brent St. Onge

**Jayme Stabler, Andy Dicks, LSB105, 10:30 - 11:20**

Synthetic Routes to Silicone-Modified Soybean Oil Copolymers  
Synthesis and polymerization of a norbornene-functionalized, photo-protected strained alkyne  
Relative Stability of Hexacarbonyldicobalt Propargylic Carbocations - Effect of Remote Substitution

**Organic III**

Patrick Cheung  
Milosz Brzozowski  
Mackenzie Thompson  
Weike Liang

**Arturo Orellana, Hovig Kouyoumdjian, LSB106, 10:30 - 11:50**

Synthesis of hydrogels polyacrylamide and polyvinylpyrrolidone cross-linked with N-methylenebisacrylamide with novel initiator system  
Synthesis of a Small Novel Thiol-Specific Fluorescent Probe: N-(1,4-dimercaptobutan-2-yl)-5-(dimethylamino)naphthalene-1-sulfonamide  
Synthesis and Purification of the Analgesic Neuropeptide Neurotensin and Three Aromatically Substituted Analogues  
Amino Acid Molecular Recognition by Boron Complex

**Organic IV**

Nicole LeGrow  
Kyle Jackman  
Denise Peda  
Advait Desai

**Shegufa Mervchant, Andrei Nikolev, LSB103, 1:40 - 3:00**

Synthesis and Self-Assembly of Discotic Triphenylenes bearing Imide Groups.  
Designing a Ligand for Long-lifetime Ethylene Polymerization with Polar Co-Monomers  
Synthesis of Conjugated Poly(3-hexylthiophene)-Poly(3-hexylselenophene) Comb Copolymers Using a "Graft-To" Approach  
Solvent Effects on the Stereoselectivity of Aprotic Glycosylations

<b>Organic V</b>	<b>Jayme Stabler, Andy Dicks, LSB105, 1:40 - 3:00</b>
Natalie Liang	Cyclen Derived Re(I)/99mTc(I) Tricarbonyl Complexes Towards the Development of Imaging Agents for CXCR4
Piryanka Sasidharan	Development of Gd-free MRI contrast agents by use of Mn(III) porphyrins
Ryan Moreira	Facile Oxidative Ring Opening of Benzothiazoles
Sherif Meshref	Metal Fullerene Cluster
<b>Organic VI</b>	<b>Arturo Orellana, Hovig Kouyoumdjian, LSB106, 1:40 - 3:00</b>
Mohamad Harb	Ring-Size Effects On Structures And Properties Of Benzo-fused Dithiazolyl Radicals
Michael Maximino	The Synthesis of Hexahydropyridazine Derivatives Through the [4+2] Cycloaddition of Donor-Acceptor Cyclobutanes and cis-Diazenes
Troy Babcock	Synthesis of bis(phosphine) and diaryl germylene to investigate P-H bond activation
Rose Anne Fayoumi	Self-Destructing Polymers: Creating Thermally Sensitive End-Caps
<b>Organic VII</b>	<b>Shegufa Mervchant, Andrei Nikolev, LSB103, 3:30 - 4:50</b>
Gillian Hawes	Optimization of the Alignment and Sorting of Single-Walled Carbon Nanotubes
Anthony Antoniani	Novel pentacene derivatives with fused thiophene rings as potential semiconducting materials
Tatiana Rogova	Multicomponent Reactions with Amphoteric $\alpha$ -Borylaldehydes: A Novel Route to Boron-Containing Molecules and Peptide Macrocycles
Matthew Baistrocchi	Synthesis of a Kartogenin Conjugated Poly(ester amide) for the Improved Treatment of Osteoarthritis
<b>Organic VIII</b>	<b>Jayme Stabler, Andy Dicks, LSB105, 3:30 - 5:10</b>
Steven Rhodes	Cu-Catalyzed one-pot atom economical synthesis of pyrido[4,3-b]indoles using 2-bromo-3-formylindoles and phenylacetylenes
Selvyn Simoes	Synthesis of Sulfur Containing Triphenylamine Based Dyes for Dye Sensitized Solar Cell Applications
Victoria Marando	Efficient Synthesis of Carborane-Containing Dendrons for Boron Neutron Capture Therapy
Albert Gevorkian	Temperature-Responsive Supramolecular Nanofibrillar Hydrogels for Cell Encapsulation Growth and Release
Jordan Bentley	BODIPY Phos-faux-lipids: Synthesis of a Novel BODIPY Fatty Acid

## Physical / Other

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<b>Other I</b>	<b>Al-Amin Dhirani, Rudy Majumdar, PS317, 10:30 - 11:50</b>
Kyle Vollett	Effect of sugar and processing on the viscosity profiles of palm oils during crystallization
Adrian Argudo	Analysis of confectioner's sugar and cooling rate on palm oil ripening by multiple regression
Melinda Dass	The effect of droplet size and interfacial structure of water-in-oil fat crystal stabilized emulsions on shelf stability
Daniel Trajanoski	Self-Launching of Hyperbolic Phonon Polaritons in Hexagonal Boron Nitride
<b>Other II</b>	<b>Al-Amin Dhirani, Rudy Majumdar, PS317, 1:40 - 3:00</b>
Malek El-Aooiti	A study of the crystallization and competitive adsorption to the water-oil interface using axisymmetric drop shape analysis
Brianne Potts	Turning Back Time - Characterization of Nineteenth Century Daguerreotypes in the Twenty First Century
Hayden Foy	Tuning the Optical Properties of Plasmonic Nanostructures
Austin Lindquist	Application of Optimal Control Theory to Solid-State NMR for the Acquisition of Ultra-Wideline NMR Spectra
<b>Other III</b>	<b>Al-Amin Dhirani, Rudy Majumdar, PS317, 3:30 - 5:10</b>
Austin Peach	<sup>35</sup> Cl Solid-State NMR Spectroscopy of Fluoxetine HCl Cocrystals
Jacqueline E. Gemus	Characterization of Mixed Linker Zeolitic Imidizolate Frameworks via Solid-State Nuclear Magnetic Resonance
Michael Leslie	The fate of isocyanic acid (HNCO): investigation into possible sinks within the atmosphere
Jake Burner	Investigation of the unimolecular reactions of nitro-substituted polycyclic aromatic hydrocarbons
Andre Castillo	The Shelf Stability of a 20% water-in-oil Emulsion Influenced by Surfactants, Water Droplet Size and the Presence of a Fat Crystal Network

5:10 - End Sessions

6:00 - 9:00 - Banquet, The Underground

**END**