2018 ACA Annual Meeting

Program Chair ............................................ Gerald Audette
Program Chair ............................................ Tiffany Kinnibrugh
Poster Chair ............................................. Louise Dawe
Poster Chair ............................................. David Rose

Council 2018
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Chief Financial Officer .. Narasinga Rao

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Communications .......... Katrina Forest
Education .................. Andy Howard
Data, Standards .......... Stephen Burley

SIG Chairs 2018
Best Practices ............... Nicholas Sauter
BioMac ....................... Elizabeth Goldsmith
Cryo-EM ..................... Catherine Lawson
Fiber Diffraction .......... Paul Langan
General Interest .......... Mike Takase
Industrial ............... Anna Gardberg
Light Sources ............... Ray Sierra
Materials Science .... Karena Chapman
Neutron Scattering ...... Brent Melot
Powder Diffraction ...... Daniel Shoemaker
Service ...................... Jeff Bacon
Small Angle Scattering . Thomas Weiss
Small Molecules .......... Graciela Diaz deDelgado
Young Scientists .......... Chelsy Chesterman

Diamond
Anatrace/ Molecular Dimensions
Art Robbins Instruments
Bruker AXS Inc.
Rigaku/Oxford Diffraction
Stoe & Cie GmbH
TTP Labtech Ltd.

Emerald
ATPS Inc.
Cambridge Cryst Data Ctr.
Charles Supper Company
Cryo Industries Of America Inc.
Formulatrix
International Center for Diffraction Data
PROTO Manufacturing Ltd.
Rayonix LLC

Ruby
Anton Paar GmbH
Dectris Ltd.

2018 ACA Corporate Members
The ACA is proud to acknowledge the following organizations for their generous support of the 2018 Annual Meeting.

**MEETING SPONSORS**

Diamond [$5,000+]

- Bruker
- IUCr

Ruby [$2,500 - $4,999]

- Gatan
- MitteGen

Emerald [$1,000 - $2,499]

- Anton Paar
- Dectris
- Hampton Research
- Leica Microsystems
- MSA
- Oak Ridge National Lab

- Pittsburgh Diffraction Society
- Poly Crystallography INC.
- Rigaku Americas Corp
- Wyatt Technology Group
- Xenocs

Sapphire [Up to $999]

- Anatrace/Molecular Dimensions
- ChemMatCARS
- Crystals
- Douglas Instruments
- G.L. Clark X-ray Facility
- GenScript Inc
- HKL Research Inc.
- IDT Inc
- Malvern Instruments Inc.
- PROTO X-Ray Diffraction
- Stoe & Cie GmbH
- Thermo Fischer
- TTP Labtach
- University at Buffalo
- University of Minnesota
- VWR
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Selected Values of the Crystallographic Properties of the Elements

This reference book presents a unique and comprehensive review of the crystallographic properties of all the elements and will be a valuable resource for metallurgists and crystallographers.

VIEW A SAMPLE CHAPTER AND ORDER TODAY:
www.asminternational.org/05244G | 800.336.5152
MEETING EXHIBITORS

Exhibit Hall Hours:
Friday, July 20th from 7:30 p.m. to 10:30 p.m. [Show Closed from 12:00 p.m. to 2:00 p.m.]
Saturday, July 21st from 10:00 a.m. to 7:30 p.m. [Show Closed from 12:00 p.m. to 2:00 p.m.]
Sunday, July 22nd from 10:00 a.m. to 7:30 p.m. [Show Closed from 12:00 p.m. to 2:00 p.m.]

Vendor Passport
This year select vendors are participating in a Vendor Passport contest. To be eligible for the $50 drawings, please complete all stops on the passport (issued at the registration desk) and return it by noon on July 23, 2018 to the ACA registration desk. The drawing will be held at 6:00 P.M. on July 23, 2018.
MEETING EXHIBITORS

Exhibit Hall Hours:
- Friday, July 20th from 7:30 p.m. to 10:30 p.m. [Show Closed from 12:00 p.m. to 2:00 p.m.]
- Saturday, July 21st from 10:00 a.m. to 7:30 p.m. [Show Closed from 12:00 p.m. to 2:00 p.m.]
- Sunday, July 22nd from 10:00 a.m. to 7:30 p.m. [Show Closed from 12:00 p.m. to 2:00 p.m.]
Prof. John Polanyi is a faculty member and Nobel laureate, Dept. of Chemistry, University of Toronto, where his research group studies the molecular motions in chemical reactions. He is a Member of the Queen’s Privy Council for Canada, a Fellow of the Royal Society of Canada, and of the Royal Societies of London and of Edinburgh, a Fellow of the American Academy of Arts and Letters, and of the U.S. National Academy of Sciences, and a Fellow of the Pontifical Academy of Rome, the Russian Academy of Sciences and the Indian Academy of Science. He has served on the Prime Minister of Canada’s Advisory Board on Science and Technology. Founding Chairman of the Canadian Pugwash Group, and has written widely on science policy and the control of armaments.

John C. Polanyi Department of Chemistry University of Toronto 80 St. George Street Toronto, Ontario, M5S 3H6 CANADA Tel. No.: (416) 978-3580 Fax No.: (416) 978-7580 E-mail: jpolanyi@chem.utoronto.ca URL: http://sites.utoronto.ca/jpolanyi

Natasha Myers is an Associate Professor in the Department of Anthropology at York University, the convenor of the Politics of Evidence Working Group, director of the Plant Studies Collaboratory, and on the editorial board of the journal Catalyst: Feminism, Theory, Technoscience.

Natasha Myers, 2032 Vari Hall, 4700 Keele Street, Toronto, Ontario M3J 1P3 Canada Telephone: (416) 736-2100 x 22394 Fax: (416) 736-5768 Email: nmyers@yorku.ca URL: https://natashamyers.wordpress.com/
AWARDS

American Crystallographic Association

2018 Award Winners

2018 Martin J. Buerger Award

**Frank C. Hawthorne**
Distinguished Professor of Geological Sciences
University of Manitoba

*When: Monday, July 23rd @ 8:00 AM
Where: Grand Centre*

2018 Bertram Warren Award

**Simon Billinge**
Professor of Applied Physics, Applied Mathematics and Materials Science,
Columbia University
Scientist at Brookhaven National Laboratory

*When: Sunday, July 22nd @ 8:00 AM
Where: Grand Centre*

2018 Etter Early Career Award

**Jason McLellan**
Assistant Professor of Biochemistry
Geisel School of Medicine
Dartmouth College

*When: Tuesday, July 24th @ 8:00 AM
Where: Grand Centre*
GENERAL INFORMATION

CONFERENCE VENUE
Sheraton Centre Toronto Hotel
123 Queen Street West
Toronto, ON, M5H 2M9, Canada
(416) 361-1000

REGISTRATION HOURS
The registration desk will be open as follows:

<table>
<thead>
<tr>
<th>Day</th>
<th>Hours</th>
</tr>
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<tbody>
<tr>
<td>Friday</td>
<td>7:30 AM - 7:30 PM</td>
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<tr>
<td>Saturday</td>
<td>7:30 AM - 5:00 PM</td>
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<tr>
<td>Sunday</td>
<td>7:30 AM - 5:00 PM</td>
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<tr>
<td>Monday</td>
<td>7:30 AM - 5:00 PM</td>
</tr>
<tr>
<td>Tuesday</td>
<td>7:30 AM - 12:00 PM</td>
</tr>
</tbody>
</table>

Please make sure to check in, get your badge and exchange your banquet ticket!

EXHIBIT SHOW
The Exhibit Show is located in Osgoode & SHall A-F and will be open according to the following schedule:

<table>
<thead>
<tr>
<th>Day</th>
<th>Hours</th>
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<tbody>
<tr>
<td>Friday</td>
<td>7:30 p.m. to 10:30 p.m. [Show Closed from 12:00 p.m. to 200 p.m.]</td>
</tr>
<tr>
<td>Saturday</td>
<td>10:00 a.m. to 7:30 p.m. [Show Closed from 12:00 p.m. to 200 p.m.]</td>
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COFFEE BREAKS
The ACA will offer complimentary coffee breaks to attendees in the exhibit hall (Osgoode & SHall A-F) on Saturday, Sunday and Monday each day in the morning from 10:00 AM to 10:30 AM and in the afternoon from 3:00 PM to 3:30 PM. On Tuesday the morning coffee break will be from 10:00 AM to 10:30 AM again in the exhibit hall but the afternoon coffee break will take place in Grand Foyer at 3:00 PM to 3:30 PM.

WIRELESS CONNECTION
Network: SHERATON_MEETINGS
Access Code: aca2018

SOCIAL MEDIA
Facebook: AmerCrystalAssn
Twitter: @ACAxtal
Twitter Hashtag: #ACAToronto

GUEST MEET-UP
On Saturday, July 21st there will be a meeting from 8:00 AM to 9:00 AM in the Pine Room for guests of attendees to meet and coordinate offsite activities and plans.

COUNCIL MEETINGS
The annual Council Meeting and any additional meetings scheduled with Council will be located in the VIP Room.
GENERAL INFORMATION

**Speaker Ready Room & Talk Preparation**

The ACA will provide a separate room for speakers to review their talk and confirm that their presentation projects correctly. This room will be equipped with a laptop PC running Windows and PowerPoint and a projector. It is mandatory that speakers review their materials the day before the presentation. If you plan on connecting a Mac, be sure to bring the proper cord.

Each session room will be equipped with an LCD projector and laptop. Presenters are encouraged to bring their talk on a memory stick and to use the provided laptop. Please arrive at your session room 30 minutes before the session begins or during the coffee break to connect computers and/or copy files to the available laptop.

**Abstract / Poster Listings**

You can locate the abstract/poster listing book online: https://acaonline.secure-platform.com/a/gallery?roundId=1.

Dates and times of talks can also be found in the online program: https://acaonline.secure-platform.com/a/page/online-program.

**SIG Meetings**

**Cryo-EM**
Monday, July 23rd @ 12:00 P.M.
[Location: Grand Centre]

**Service & Small Molecule: Joint Meeting**
Monday, July 23rd @ 12:00 P.M.
[Location: Provincial South]

**Small Angle Scattering**
Monday, July 23rd @ 12:00 P.M.
[Location: Grand East]

**Canadian Division**
Saturday, July 21st @ 12:00 P.M.
[Location: Grand West]

**General Interest**
Saturday, July 21st @ 12:00 P.M.
[Location: Provincial South]

**Industrial**
Saturday, July 21st @ 12:00 P.M.
[Location: Grand East]

**Light Sources**
Saturday, July 21st @ 12:00 P.M.
[Location: Grand Centre]

**Best Practices for Data Analysis & Archiving**
Saturday, July 21st @ 5:00 P.M.
[Location: Provincial North]

**Fiber Diffraction**
Saturday, July 21st @ 5:00 P.M.
[Location: Provincial South]

**Biological Macromolecules**
Sunday, July 22nd @ 5:00 P.M.
[Location: Grand Centre]

**Materials, Neutron & Powder: Joint Meeting**
Sunday, July 22nd @ 5:00 P.M.
[Location: Provincial North]

**Young Scientists’**
Sunday, July 22nd @ 5:00 P.M.
[Location: Grand West]
Workshop No. 1: Cryo-EM - A Guide to High Resolution Structure Determination
Sponsored By: Douglas Instruments, Gatan & ThermoFisher
Chairs: Wah Chiu, Lori Passmore & John Rubinstein
Location: Provincial North
Times: 8:30 AM - 6:00 PM

Over the past five years, cryo-EM has become increasingly popular and is now the method of choice for structure determination of proteins larger than ~200 kDa. It has been particularly successful for proteins that are difficult to crystallize, including membrane proteins, large assemblies and multi-protein complexes. The aim of this workshop is to provide a detailed overview of cryo-EM specimen preparation, image processing and building/refinement of atomic models. The workshop will focus on high-resolution single particle cryo-EM. Aspects of image processing and modelling will be hands-on - state-the-art programs will be used by the students to process sample datasets.

User facilities are being established in many universities and these will allow a larger community to access cryo-EM. By teaching the main concepts and challenges in each step, this workshop will benefit those who want to use cryo-EM in the future, or who have recently transitioned into it. The organizers are experts in the topics they will be teaching and all have been involved in methods development. We will strive to include up-to-date discussions of cutting-edge methods and technology.

The tutorial by Corey Hryc will require Chimera to visualize both map and model and perform slight alterations of the data. In addition, Phenix (command line tools) will be used to optimize the molecular model with respect to the experimental data. Finally, EMAN2 will be needed to perform validation routines such as computing map/model FSC.

Chimera: https://www.cgl.ucsf.edu/chimera/
Phenix: https://www.phenix-online.org/
EMAN2: http://blake.bcm.edu/emanwiki/

Personal computers can be used and these software packages are available on Mac, Linux and Windows.

**SCHEDULE**

<table>
<thead>
<tr>
<th>Time</th>
<th>Activity</th>
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<tbody>
<tr>
<td>8:30 AM</td>
<td>Start</td>
</tr>
<tr>
<td>10:45-11:15 AM</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>12:30-1:30 PM</td>
<td>Lunch</td>
</tr>
<tr>
<td>3:15-3:45 PM</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>6:00 PM</td>
<td>End</td>
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</table>
Workshop No. 2: Molecular Art & Animation in 3D  
Chair: Chelsy C. Chesterman  
Location: Provincial South  
Times: 8:30 AM - 6:00 PM

Beautiful figures and animations have become synonymous with the publication of structural data in top research journals. Demonstrating molecular concepts and structural data using these strategies is also highly effective in scientific presentations or outreach activities. Many crystallographers enter the field with a background in biology or chemistry and are unfamiliar with creating such artwork. This workshop will focus on the creation of figures and animations in multiple software programs including PyMOL, Chimera, Blender 3D, and Maya. Topics will include factors to consider when designing your art and animations, basic operation of these programs, and follow-along examples. The main goal of the workshop will be to give participants an overview of the available tools so that they can start to explore creating their own molecular art.

Software required will be PyMOL, Chimera, Blender 3D, Maya, and Molecular Maya and participants will use their personal computers. These programs are free or have a free educational version. Installation instructions will be distributed to participants by e-mail prior to the workshop and participants will be asked to install as much as they can ahead of time. Many of these programs will benefit from using a 3-button mouse not available on most laptops. Participants are asked to bring their own mouse.

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<th>Time</th>
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<tr>
<td>8:30 AM</td>
<td>Start</td>
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<tr>
<td>10:30-10:45 AM</td>
<td>Coffee Break</td>
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<tr>
<td>11:30-12:30 PM</td>
<td>Lunch (On Your Own)</td>
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<tr>
<td>3:00-3:30 PM</td>
<td>Coffee Break</td>
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<td>6:00 PM</td>
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Workshop No. 4: Applications of Small Angle Scattering to Structural Biology: An Introduction
Sponsored By: Anton Paar, Rigaku, Wyatt Technology & Xenoxs
Chairs: Kushol Gupta, Richard Gillilan, Jesse Hopkins, Haydyn Mertens & Srinivas Chakravarthy
Location: Chestnut West
Times: 8:00 AM - 5:30 PM

Over the past two decades, SAS has become a mainstay technique for the study of structure and composition in solution for structural biologists around the world. In contrast to the more intensive SAS courses in Europe that extend across several days, this single-day workshop will be comprised of carefully constructed lectures and tutorials to serve as an introduction to investigators new to the technique. The workshop format will include lectures and a selection of hands-on practical exercises.

Throughout the workshop the emphasis will be on practical application: knowing how to judge data quality, how to troubleshoot during data collection, and the expectations for a successful experiment and acceptable publication. Students will also learn about aspects of home laboratory data collection and will be introduced to experiments at national user facilities (synchrotrons and research reactors).

Students will be expected to bring laptops with the appropriate pre-installed software. Extra laptops will be provided in case of unexpected hardware or software issues on-site, and network connectivity will be provided as part of the course, as some exercises and tutorials will reply on external computer-server resources. Preloaded portable disks and memory sticks will be provided to help reduce the need for large downloads over conference bandwidth.

SCHEDULE

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<td>8:00 AM</td>
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<td>10:00-10:15 AM</td>
<td>Coffee Break</td>
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<tr>
<td>12:00-1:00 PM</td>
<td>Lunch</td>
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<td>3:15-3:30 PM</td>
<td>Coffee Break</td>
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<td>5:30 PM</td>
<td>End</td>
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</table>
Workshop No. 5: Rietveld Refinement And Pair Distribution Function Analyses Of In Situ X-Ray Scattering Data Within GSAS-II

Sponsored By: Argonne National Laboratory
Chairs: Olaf J. Borkiewicz
Location: City Hall Room
Times: 8:30 AM - 6:00 PM

This workshop will be a foray into structural analysis of powder X-ray scattering data - one of the most comprehensive and powerful tools for evaluating crystal structures. The primary goal of this workshop will be to discuss and explain all typical steps involved in structural analysis of X-ray scattering data with emphasis on data collected at modern users’ facilities using large-area detectors. These will include such aspects of the experiment as measurement calibration, data reduction, peak profile fitting, Rietveld refinement and others. In addition to “classic” single pattern refinement approach, we will explore strategies for handling large data sets, i.e. sequential refinements and parametric fitting to in situ and operando data. Part of the workshop will be also dedicated to the complementary use of pair distribution function (PDF) analysis, which allow extraction of structural information from amorphous and disordered materials, for which classical crystallographic approaches may not yield satisfactory results. All tasks pertaining to the workshop will be accomplished within General Structure Analysis System (GSAS-II).

GSAS-II is a powerful open-source Python-based tool that addresses all types of crystallographic studies and handles all standard activities involved in the reduction and analysis of data acquired with both X-ray and neutron probes. This will be an excellent opportunity to learn how to take full advantage of this powerful software directly from the program authors, Robert Von Dreele and Brian Toby, and how to apply this knowledge to real-world applications and experimental data sets presented by beamline scientists, Kamila Wiaderek, Andrey Yakovenko and Olaf Borkiewicz, Advanced Photon Source, Argonne National Laboratory.

**SCHEDULE**

<table>
<thead>
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<tbody>
<tr>
<td>8:30 AM</td>
<td>Start</td>
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<tr>
<td>9:40 - 9:50 AM</td>
<td>Coffee Break</td>
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<tr>
<td>11:30 - 1:00 PM</td>
<td>Lunch</td>
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<tr>
<td>2:15-2:30 PM</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>6:00 PM</td>
<td>End</td>
</tr>
</tbody>
</table>
**TMT1 - Three Minute Thesis (1)**

**Chairs: Victor Young & Juhas Pavol**

**Room: Provincial North**

**Scheduled Time: 08:00**

- **Structural Investigation of a Novel Copper(II) Complex with Pyridoxal Thiosemicarbazone.** Marcio Adriano Sousa Chagas.

**Scheduled Time: 08:03**

- **Chiral Segregation of Space by Anionic Assemblies found in Tartramide-based Spiroborate Salts.** Aristyo Soecipto.

**Scheduled Time: 08:06**


**Scheduled Time: 08:09**

- **NMR Crystallographic Insights into the Structures of Difficult to Characterize Materials.** Giovanna Pope.

**Scheduled Time: 08:12**

- **Overexpression, purification of GSK3 and its interaction with an inhibitory fragment of the psychiatric risk protein DISC1.** Narsimha Pujari.

**Scheduled Time: 08:15**

- **Structural investigation of the oligomeric domain of the psychiatric risk protein DISC1.** Anand Nambisan.

**Scheduled Time: 08:18**

- **Structural characterization of a novel amino acid decarboxylase.** Raquel Sofia Correia Cordeiro.

**Scheduled Time: 08:21**

- **Structural delineation of human antibody responses against malaria transmission-blocking vaccine antigen Pfs25.** Brandon McLeod.

**Scheduled Time: 08:24**

- **Structural insights into the dimeric human PNPase revealing why the disease-linked mutants exhibit lower RNA import and degradation activities.** Bagher Golzarroshan.
SATURDAY | JULY 21

Scheduled Time: 08:27
Determining the mechanism of LINE-1 ribonucleoprotein particle assembly and inhibition by nucleoside reverse transcriptase inhibitors. Jocelyn Newton.

Scheduled Time: 08:30
Acidochromic Spiropyran-Merocyanine stabilisation in the solid state. Vanessa Kristina Seiler.

Scheduled Time: 08:33
Structural Determinants for the Activation of Soluble Guanylyl Cyclase. Kenneth Childers.

Scheduled Time: 08:36
EM studies of cytochrome bc1 to elucidate inhibitor binding. Rachel Johnson.

Scheduled Time: 08:39
Conformational flexibility of pore loop-1 gives insights into substrate translocation by AAA+ protease FtsH. Matthias Uthoff.

Scheduled Time: 08:42
Self-Assembled Three-Dimensional Deoxyribonucleic Acid (DNA) Crystals. Yue Zhao.

Scheduled Time: 08:45

TMT1A - Three Minute Thesis (1A)
Chairs: Victor Young & Juhas Pavol
Room: Provincial South

Scheduled Time: 08:00
Atomic-level perspective on the functionality of nanoalloy catalysts inside operating fuel cells by combined in-operando high energy x-ray spectroscopy and total scattering. Yazan Maswadeh.

Scheduled Time: 08:03
In-situ measurement of atomic displacement in TiO2 during flash sintering experiments. Bola Yoon.

Scheduled Time: 08:06

Scheduled Time: 08:09
Mechanistic underpinnings of allostery, catalysis and domain synchronization in an ammonia tunneling enzyme. Santosh Shivakumaraswamy.

Scheduled Time: 08:12

Scheduled Time: 08:15
Structure and Function of Terfesatin Biosynthesis Proteins TerB and TerC. Jonathan Clinger.

Scheduled Time: 08:18
Diverse ligand-binding domain combinations at the distal end of bacterial RTX adhesins are postal codes for biofilm formation. Tyler Vance.

Scheduled Time: 08:21
Structural Basis of Conserved Flagellin-mediated TLR5 Stimulation. Wanseok Song.

Scheduled Time: 08:24
Evidence for Breathing of a Class I Fusion Protein at the Cell Surface. Morgan Gilman.
<table>
<thead>
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<tbody>
<tr>
<td>Scheduled Time: 08:30</td>
<td>Role of AlgL in Pseudomonas aeruginosa alginate biosynthesis. Andreea Gheorghita.</td>
</tr>
<tr>
<td>Scheduled Time: 08:33</td>
<td>The molecular mechanism of the type IVa pilus motor. Matthew McCallum.</td>
</tr>
<tr>
<td>Scheduled Time: 08:39</td>
<td>Crystallization and structural studies of an aldo-keto reductase from opium poppy. Miguel Torres.</td>
</tr>
<tr>
<td>T1: Transactions 1 - Shining a Light on Structure-Based Drug Design</td>
<td>Chairs: Steve Sossion &amp; Vincent Stoll</td>
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<tr>
<td>Room: Grand Centre</td>
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<tr>
<td>Scheduled Time: 9:30 AM</td>
<td>IMCA-CAT: Accelerating Drug Discovery Through Synchrotron-Based Structural Biology</td>
</tr>
<tr>
<td>Lisa J. Keefe</td>
<td>IMCA-CAT / HWI</td>
</tr>
<tr>
<td>Scheduled Time: 10:00 AM</td>
<td>Systematic analysis of atomic protein-ligand interactions in the PDB</td>
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<tr>
<td>Matthieu Schapira</td>
<td>Structural Genomics Consortium</td>
</tr>
<tr>
<td>Scheduled Time: 11:00 AM</td>
<td>X-ray Free Electron Laser: Opportunities for drug discovery</td>
</tr>
<tr>
<td>Michael Hennig</td>
<td>LeadXpro AG</td>
</tr>
<tr>
<td>Scheduled Time: 11:30 AM</td>
<td>Achieving higher performance in high-throughput compound and fragment screening campaigns by the use of “Club Class” data collection with Pipedream and CRIMS</td>
</tr>
<tr>
<td>Gerard Bricogne</td>
<td>Global Phasing Limited</td>
</tr>
<tr>
<td>Scheduled Time: 12:00 PM</td>
<td>Using small molecule crystal structure data to improve drug discovery</td>
</tr>
<tr>
<td>Jason Cole</td>
<td>Cambridge Crystallographic Data Centre</td>
</tr>
<tr>
<td>T2: Transactions 2 - Shining a Light on Structure-Based Drug Design</td>
<td>Chairs: Steve Sossion &amp; Vincent Stoll</td>
</tr>
<tr>
<td>Room: Grand Centre</td>
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<tr>
<td>Scheduled Time: 1:30 PM</td>
<td>Structure of HIV-1 TAR in Complex with a Lab-Evolved Protein Provides Insight into RNA Recognition and Synthesis of a Constrained Peptide that Impairs Transcription</td>
</tr>
<tr>
<td>Joseph Wedekind</td>
<td>University of Rochester School of Medicine &amp; Dentistry</td>
</tr>
<tr>
<td>Scheduled Time: 2:00 PM</td>
<td>Fragment screening for a protein-protein interaction inhibitor to WDR5</td>
</tr>
<tr>
<td>Thomas Peat, CSIRO</td>
<td></td>
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<tr>
<td>Scheduled Time: 2:30 PM</td>
<td>Make the right measurement – discovery of an allosteric inhibition site for p300-HAT</td>
</tr>
<tr>
<td>Anna Gardberg</td>
<td>Constellation Pharmaceuticals</td>
</tr>
</tbody>
</table>
Functional optimization of agonistic antibodies to OX40 receptor with novel Fc mutations to promote antibody multimerization

Mark J. Chiu
Eli Lilly Research & Development

Development of small molecule inhibitors that target protein-protein interactions in a transcription factor.

Gil Privé
Princess Margaret Cancer Centre

CryoEM for drug discovery, design, understanding and application.

Giovanna Scapin
Merck & Co., Inc.

1.1.1 Closing the R-Factor Gap in Protein Crystallography

Chairs: James Holton & Robert Thorne
Room: Grand West

On the information content of X-ray diffraction data. Randy Read & Robert Oeffner.

Improved chemistry restraints for crystallographic refinement by integrating Amber molecular mechanics in Phenix. David Case & Pqwel Janowski.

On behaviour of statistical reliability indicators during crystal structure refinement. Garib Murshudov.

How many conformers do you need?. James Holton.

Better bulk-solvent models can improve model-to-data fit. Pavel Afonine.

qFit-ligand reveals widespread configurational heterogeneity of drug-like molecules in X-ray electron density maps. Henry van den Bedem.

Correlated Motions from Protein Crystallography. Steve Meisburger & David Case.

Vagabond: a new project for macromolecular model refinement. Helen Ginn.

1.1.2 Structural biology of nucleic acids and protein-nucleic acid complexes

Chairs: Joseph E. Wedekind, Rui Zhao & Aaron Robart
Room: Grand East


Structural and biochemical analyses of PadR-mediated transcriptional regulation. Sun Cheol Park.
Scheduled Time: 9:35 AM  
Duration: 25 Minutes  

Scheduled Time: 10:30 AM  
Duration: 25 Minutes  

Scheduled Time: 10:55 AM  
Duration: 20 Minutes  
Architecture of the U6 snRNP reveals specific recognition of 3-end processed U6 snRNA. Eric Montemayor & Allison Didychuk.

Scheduled Time: 11:15 AM  
Duration: 20 Minutes  
Regulating bacterial gene expression with small molecules by altering DNA supercoiling. Soumya G Remesh & Subhas Verma.

Scheduled Time: 11:35 AM  
Duration: 25 Minutes  
Spacer acquisition mechanism in type II-A CRISPR system. Ailong Ke & Yiebi Xiao.

1.1.3 Dynamic Crystals as Molecular Materials  
Chairs: Dmitriy V. Soldatov & Louise Dawe  
Room: Provincial North

Scheduled Time: 9:00 AM  
Duration: 30 Minutes  

1.1.4 Neutron and X-ray Scattering of Correlated and Quantum Materials  
Chairs: J.E. Greedan & Craig Bridges  
Room: Provincial South

Scheduled Time: 9:30 AM  
Duration: 15 Minutes  

Scheduled Time: 9:45 AM  
Duration: 15 Minutes  

Scheduled Time: 10:30 AM  
Duration: 20 Minutes  

Scheduled Time: 10:50 AM  
Duration: 30 Minutes  

Scheduled Time: 11:20 AM  
Duration: 20 Minutes  
Understanding the stepwise mechanism in the formation of halogen-bonded organic cocrystals by mechanochemistry. Filip Topi & Poppy Hindle.

Scheduled Time: 11:40 AM  
Duration: 20 Minutes  
Dithienylethene Based Crystalline Solids. Travis Mitchell & Dinesh (Dan) Patel.
SATURDAY | JULY 21

Scheduled Time: 9:00 AM
Duration: 30 Minutes

Scheduled Time: 9:30 AM
Duration: 15 Minutes

Scheduled Time: 9:45 AM
Duration: 15 Minutes
Long range versus short range spin correlations in A0.8La1.2MnO4.1 (A = Sr, Ba). Mirela Dragomir.

Scheduled Time: 10:30 AM
Duration: 20 Minutes

Scheduled Time: 10:50 AM
Duration: 30 Minutes
Magnetic order and spin dynamics of jeff = _ Ir4+ moments on the fcc lattice in La2BirO6 (B = Mg, Zn). Adam Aczel.

Scheduled Time: 11:20 AM
Duration: 20 Minutes
Magnetic Moment Fragmentation in Nd2ScNbO7. Christopher Wiebe.

Scheduled Time: 11:40 AM
Duration: 20 Minutes
Dy2ScNbO7: an unconventional spin ice?. Megan Rutherford.

**1.2.1 Structural Dynamics - In honour of Phil Coppens**
**Chairs: Yu-Sheng Chen & Jason Benedict**
**Room: Grand East**

Scheduled Time: 1:35 PM
Duration: 25 Minutes
From Structure to Structural Dynamics. Majed Chergui.

Scheduled Time: 2:00 PM
Duration: 25 Minutes
First crystallography experiments at the European XFEL. Marc Messerschmidt.

Scheduled Time: 2:25 PM
Duration: 25 Minutes
Ultrafast Reaction Pathways in a Metalloprotein Revealed by Optical Polarization Selected X-ray Transient Absorption Spectroscopy and Quantum Mechanical Calculations. Lin Chen.

Scheduled Time: 3:20 PM
Duration: 25 Minutes

Scheduled Time: 3:45 PM
Duration: 15 Minutes

Scheduled Time: 4:00 PM
Duration: 25 Minutes
Dancing in a Chemical Graveyard. Tomislav Friscic.

Scheduled Time: 4:25 PM
Duration: 10 Minutes

Scheduled Time: 4:35 PM
Duration: 15 Minutes
The magnitude of quanta from variance and intensity measurements. Wilfred Fullagar & Andrew Kingston.
1.2.2 Hybrid Techniques
Chairs: Bhushan Nagar & Srinivas Chakravart
Room: Provincial North

Solving the phase problem in solution scattering. Thomas Grant.

Scheduled Time: 1:35 PM
Duration: 25 Minutes


Scheduled Time: 2:00 PM
Duration: 20 Minutes

Accurately characterizing protein assembly states in solution with a combination of size exclusion chromatography (SEC), multi-angle light scattering (MALS) and small angle X-ray scattering (SAXS). Zhen Xu & Lokesh Gakhar.

Scheduled Time: 2:20 PM
Duration: 20 Minutes

Exploring the landscape of biological solutions with the BioSAXS-2000nano. Angela Criswell & Mark Del Campo.

Scheduled Time: 2:40 PM
Duration: 20 Minutes


Scheduled Time: 3:00 PM
Duration: 25 Minutes

Measuring the solvent quality of water for disordered proteins from a single SAXS measurement. Tobin Sosnick & Micayla Bowman.

Scheduled Time: 3:30 PM
Duration: 20 Minutes

Structural insights into the interaction of the conserved mammalian proteins GAPR-1 and Beclin 1, a key autophagy protein. Christopher Colbert & Yue Li.

1.2.3 Neutrons as Complimentary Probes for Crystals and Scattering
Chairs: Leighton Coats & Gloria Borgstsal
Room: Grand West

Controllable Activation of Nanoscale Dynamics in a Disordered Protein Alters Binding Kinetics. Zimei Bu & David Callaway.

Scheduled Time: 1:30 PM
Duration: 30 Minutes

The missing atom in function: reliability of the determination of hydrogen positions in protein structures. Dagmar Ringe & Cheryl Kreinbring.

Scheduled Time: 2:00 PM
Duration: 30 Minutes

Neutron Diffraction Studies of Pyridoxal-5'-Phosphate Dependent Enzymes. Timothy Mueser & Steven Dajnowicz.

Scheduled Time: 2:30 PM
Duration: 20 Minutes


Scheduled Time: 3:30 PM
Duration: 20 Minutes


Scheduled Time: 3:50 PM
Duration: 20 Minutes

Observing Membrane Proteins via SANS During Lipidic Cubic Phase Crystallization. Thomas Cleveland & Paul Butler.

1.2.4 Forefront of Electron Scattering for Nanoscale and Metastable Materials / Electron Diffraction

Chairs: Jing Tao & Albina Borisovich
Room: Provincial South

Quantitative determination of polarization from 4D scanning electron diffraction experiments. Jim Ciston.


MeV Ultrafast Electron Scattering at SLAC: Status and Opportunities. Renkai Li, Suji Park.
PL1 Bertram Warren Award to Simon Billinge
Lisa J. Keefe, Presiding
Room: Grand Centre

Scheduled Time: 8:00 AM
A series of fortunate events: How the PDF method went from niche technique to mainstream and beyond.
Simon Billinge.

2.1.1 Special Sessions in Honour of Richard E. Marsh
Chairs: Louise Dawe & Mike Takase
Room: Grand West

Scheduled Time: 9:00 AM
Duration: 20 Minutes
Honoring a Great Crystallographer: Richard E. Marsh. Susan Byram

Scheduled Time: 9:20 AM
Duration: 20 Minutes

Scheduled Time: 9:40 AM
Duration: 20 Minutes
A journey through the CSD in celebration of Richard E. Marsh. Suzanna Ward & Amy Sarjeant.

Scheduled Time: 10:30 AM
Duration: 30 Minutes

Scheduled Time: 11:00 AM
Duration: 30 Minutes
My Postdoc Work with Dick Marsh at Caltech and his Participation as a Lecturer at the ACA Summer School at the University of Georgia. Bi-Cheng Wang.

Scheduled Time: 11:30 AM
Duration: 30 Minutes
Forty Years of Marshing: Is the missed Symmetry Problem Now Solved?. Anthony Spek.

2.1.2 Current state of instrumentation, automation, status and future. Focus on practical aspects.
Chairs: Matthew Clifton & Jan Abendroth
Room: Grand East

Scheduled Time: 9:00 AM
Duration: 20 Minutes
High throughput fragment screening at the nano-scale: laboratory miniaturization and beam-line integration. Alexei Soares.

Scheduled Time: 9:20 AM
Duration: 20 Minutes

Scheduled Time: 9:40 AM
Duration: 20 Minutes

Scheduled Time: 10:30 AM
Duration: 20 Minutes
Automated data collection services at ESRF Massif-1. Didier Nurizzo & Matthew Bowler.

Scheduled Time: 10:50 AM
Duration: 20 Minutes

Scheduled Time: 11:10 AM
Duration: 20 Minutes
Automated robot based systems for crystallography on beamlines and in laboratories, and other developments performed on FIP-BM30A at the ESRF. Jean-Luc Ferrer, Xavier Vernede.
### 2.1.3 NMR Crystallography
**Chairs:** Manish Mehta & Tomislav Friscic  
**Room:** Provincial South

<table>
<thead>
<tr>
<th>Scheduled Time</th>
<th>Duration</th>
<th>Title</th>
<th>Presenter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>11:15 AM</td>
<td>25 Minutes</td>
<td>What solid-state NMR can do to characterize metal-organic frameworks?</td>
<td>Yining Huang.</td>
</tr>
</tbody>
</table>

### 2.1.4 Advances in Biological Cryo-Electron Microscopy 1  
**Chairs:** Wah Chiu & Lori Passmore  
**Room:** Grand Centre

<table>
<thead>
<tr>
<th>Scheduled Time</th>
<th>Duration</th>
<th>Title</th>
<th>Presenter(s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>9:00 AM</td>
<td>30 Minutes</td>
<td>Single-Particle Cryo-EM Studies of Lipopolysaccharide Transport.</td>
<td>Maofu Liao.</td>
</tr>
<tr>
<td>9:45 AM</td>
<td>15 Minutes</td>
<td>Core components of bacterial protein secretion systems revealed at high resolution by cryo-electron microscopy.</td>
<td>Justin Deme.</td>
</tr>
<tr>
<td>10:30 AM</td>
<td>30 Minutes</td>
<td>How is electrical signal generated? Structural and mechanistic investigations of Nav channels.</td>
<td>Nieng Yan.</td>
</tr>
<tr>
<td>11:00 AM</td>
<td>15 Minutes</td>
<td>eBIC: Applying over 10yrs of software automation and support of MX beamlines to CryoEM.</td>
<td>Alun Ashton, M Basham.</td>
</tr>
</tbody>
</table>
SUNDAY | JULY 22

Scheduled Time: 11:15 AM
Duration: 45 Minutes
Near-atomic resolution CryoEM analysis of the Type III Secretion Injectisome.
Natalie Strynadka.

2.1.5 Materials for a Sustainable Future
Chairs: Mario Wriedt & Fernando J. Uribe-Romo
Room: Provincial North

Scheduled Time: 9:00 AM
Duration: 25 Minutes
In situ and operando structural analysis with high-energy X-rays at the Advanced Photon Source APS.
Uta Ruett, Olaf Borkiewicz.

Scheduled Time: 9:25 AM
Duration: 15 Minutes
Tunable Solid State Fluorescence in Isoreticular Metal Organic Frameworks.
Wesley Newsome, Fernado Uribe-Romo.

Scheduled Time: 9:40 AM
Duration: 20 Minutes
Understanding of Metal-Organic Frameworks through Mechanochemistry: From Experiment to Theory.
Tomislav Friscic.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
MOF Vaccines—Decreasing the Dependency on Refrigerated Transport.
Jeremiah Gassensmith.

2.2.1 Special Sessions in Honour of Richard E. Marsh
Chairs: Paul Boyle & Alexander Filatov
Room: Grand West

Scheduled Time: 1:30 PM
Duration: 30 Minutes
Marsh, McLuhan and the Crystallographic Message.
Larry Falvello.

Scheduled Time: 2:00 PM
Duration: 30 Minutes
Program to Find and Characterize Commensurate Modulations in Molecular Crystals.
Carolyn Brock, Robin Taylor.

Scheduled Time: 2:30 PM
Duration: 30 Minutes
Using phases to determine the space group.
George Sheldrick.

Scheduled Time: 3:30 PM
Duration: 20 Minutes
Detecting errors and inconsistencies in the structure determination of pharmaceutical compounds: wrong structures, twinning, disorder and modulation.
Gra- ciela Díaz de Delgado, María Cecilia Dávila.

Scheduled Time: 11:25 AM
Duration: 15 Minutes
Systematic Isoreticular Expansion of Titanium Metal-Organic Frameworks.
Matthew Logan, Fernando Uribe-Romo.

Scheduled Time: 11:40 AM
Duration: 20 Minutes
Hui Wu.

2.2.1 Special Sessions in Honour of Richard E. Marsh
Chairs: Paul Boyle & Alexander Filatov
Room: Grand West

Scheduled Time: 1:30 PM
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Detecting errors and inconsistencies in the structure determination of pharmaceutical compounds: wrong structures, twinning, disorder and modulation.
Gra- ciela Díaz de Delgado, María Cecilia Dávila.

Scheduled Time: 11:05 AM
Duration: 20 Minutes
Structure-property relationships in titanium-based metal-organic frameworks for the photocatalytic reduction of carbon dioxide.
Fernando Uribe-Romo.
Scheduled Time: 3:50 PM  
Duration: 20 Minutes  

Scheduled Time: 4:10 PM  
Duration: 20 Minutes  
Hypersymmetry Then and Now. Victor Young.

Scheduled Time: 4:30 PM  
Duration: 30 Minutes  
The Inverse Marsh Error. Frank Fronczek.

2.2.2 New Advances in Fiber Diffraction  
Chair: J. Orgel & P. Langan  
Room: Provincial South

Scheduled Time: 1:30 PM  
Duration: 45 Minutes  
Contemporary and ancient tissues give modern insights into biomedical engineering. Joseph Orgel.

Scheduled Time: 2:15 PM  
Duration: 45 Minutes  
MuscleX: A new tool for analyzing X-ray diffraction patterns from muscle and other fibrous systems. Thomas Irving, Jiranun Jiratrakanvong.

Scheduled Time: 3:30 PM  
Duration: 45 Minutes  
Tension wood provides insight into structural changes in biomass resulting from chemical pretreatment. Volker Urban.

Scheduled Time: 4:15 PM  
Duration: 45 Minutes  
Changes to the packing structure of type I collagen from non-enzymatic glycation. Rama Sashank Madhurapantula, Joseph Orgel.

2.2.3 General Interest - 1  
Chair: Carla Slebodnick & Soumya Remesh  
Room: Grand East

Scheduled Time: 1:30 PM  
Duration: 15 Minutes  

Scheduled Time: 1:45 PM  
Duration: 15 Minutes  
Temperature Validation using the CSD Python API. Dean Johnston, Amy Sarjeant.

Scheduled Time: 2:00 PM  
Duration: 15 Minutes  

Scheduled Time: 2:15 PM  
Duration: 15 Minutes  
Investigating conformational landscapes through alternative cryocystallographic approaches. Matt McLeod, Todd Holyoak.

Scheduled Time: 2:30 PM  
Duration: 15 Minutes  
Enhancing high-throughput detection of protein nanocrystals. Sarah Bowman, Ellen Gualtieri.

Scheduled Time: 3:30 PM  
Duration: 15 Minutes  
New Online Curriculum: The PDB Pipeline & Data Archiving. Catherine Lawson, Margaret Gabanyi.

Scheduled Time: 3:45 PM  
Duration: 15 Minutes  
Finding novel pyrophosphate-dependent kinases based on their donor selectivity determinants revealed by crystal structures. Masahiro Fujihashi, Ryuhei Nagata.
2.2.4 Advances in Biological Cryo-Electron Microscopy 2
Chairs: Wah Chiu & Lori Passmore
Room: Grand Centre

Scheduled Time: 1:30 PM
Duration: 45 Minutes
CryoEM snapshots of the spliceosome provide insights into the molecular mechanism of pre-mRNA splicing. Kiyoshi Nagai.

Scheduled Time: 2:15 PM
Duration: 15 Minutes

Scheduled Time: 2:30 PM
Duration: 30 Minutes
Molecular Therapy for 2.5-4Å Models: Anecdotes and Progress from the Cryo-EM Model Challenge. Jane Richardson, Christopher Williams.

Scheduled Time: 3:30 PM
Duration: 30 Minutes

Scheduled Time: 4:00 PM
Duration: 15 Minutes
Cryo EM structure of yeast U1 snRNP offers insight into alternative splicing. Rui Zhao, Xueni Li.

Scheduled Time: 4:15 PM
Duration: 15 Minutes
Improving 3D reconstructions of macromolecular conformations. Javier Vargas, Moshen Kazemi.

Scheduled Time: 4:30 PM
Duration: 15 Minutes
Explore Size and Resolution Limits with Conventional Cryo-EM. Gabriel Lander, Mark A. Herzik Jr.

2.2.5 The diverse world of materials chemistry: from deep space to titanium dioxide nanocomposites
Chairs: Ashfia Huq & Olaf Borkiewicz
Room: Provinicial North

Scheduled Time: 1:30 PM
Duration: 24 Minutes

Scheduled Time: 1:54 PM
Duration: 22 Minutes
Infusible Nuclear Fuel Metamaterial for Deep Cosmic-Space Explorations. Boris Udovic.

Scheduled Time: 2:16 PM
Duration: 22 Minutes
Growing mechanism and change of phase of synthesized CdSe nanoparticles. Janeth Sarmiento, Enrique Rosendo.

Scheduled Time: 3:30 PM
Duration: 18 Minutes
Custom setup for organic crystal growth by vapor deposition. Georgii Bogdanov, Sergei Rigin.

Scheduled Time: 3:48 PM
Duration: 18 Minutes
Volume isotope effect in benzene; the anisotropic thermal expansion of H/D and halogen-substituted benzene crystals. Dominic Fortes, Silvia Capelli.

Scheduled Time: 4:06 PM
Duration: 18 Minutes
Combining experimental and computational techniques for polymorph screening. Dubravka Sisak Jung, Ivan Halasz.

Scheduled Time: 4:24 PM
Duration: 18 Minutes
Computational analysis of charge-transfer crystalline complexes. Sergei Rigin, Georgii Bogdanov.
2.3.1 Would You Publish This?
Chairs: Dannielle Gray & Jeff Burtke
Room: Provincial North

Scheduled Time: 6:30 PM
Duration: 15 Minutes
Don’t throw good time after bad money. Louise Dawe, Amy Sarjeant.

Scheduled Time: 6:45 PM
Duration: 15 Minutes
Whole Molecule Disorder in the Crystal Structures of 7-Chloro & 7-Methyl Indole. Joe Tanski.

Scheduled Time: 7:00 PM
Duration: 15 Minutes
Challenging crystal structures of some iridium complexes: Disorder and twinning. Victor Young, Robert Sanner.

Scheduled Time: 7:15 PM
Duration: 15 Minutes
Deformed thoughts on tetrahedral carbonates. Christine Beavers, Cara Vennari.

Scheduled Time: 7:30 PM
Duration: 15 Minutes
Can we leave out the spaghetti? Danielle Gray, Daniel Davies.

SUNDAY EVENING ACTIVITIES

5:30 PM - 7:30 PM
SA Poster Session
[Osgoode & SHall A-F]

8:00 PM YSIG Networking Mixer

WHERE: The 3 Brewers
120 Adelaide Street West
Toronto ONT M5H 1T1

SPONSORED BY:

Join us to expand your professional network and connect with friends at our mixer for young professionals!

Sponsored in part by Bruker, the Young Scientist Mixer is one of the ACA’s most popular events and is FREE to registered Students & Post-docs (ticket required). A drink ticket and light appetizers are included with your ticket.
PL2 Martin J. Buerger Award to
Frank C. Hawthorne
Lisa J. Keefe, Presiding
Room: Grand Centre

Scheduled Time: 8:00 AM
Bond topology and structural arrangements in inorganic crystals.
Frank C. Hawthorne.

3.1.1 Structural Biology of Pathogens:
Cellular Interactions, Drug Resistance, and Immune Responses - 1
Chairs: B.V.V. Prasad, Jean-Philippe Julien & Michael Becker
Room: Grand Centre

Scheduled Time: 9:00 AM
Duration: 30 Minutes

Scheduled Time: 9:45 AM
Duration: 15 Minutes
Structural studies of human antibody responses against leading malaria vaccine antigen PfCSP. Stephen Scally.

Scheduled Time: 10:30 AM
Duration: 30 Minutes
Structure-assisted Design of Universal Vaccines and Therapeutics against Influenza Virus. Ian Wilson.

Scheduled Time: 11:00 AM
Duration: 15 Minutes

Scheduled Time: 11:15 AM
Duration: 30 Minutes
Active transport across the bacterial outer membrane: the Ton motor complex. Susan Buchanan.

3.1.2 Best practices for building, refining, and analyzing ligands in macromolecular structures
Chairs: Anna Gardberg & Kurt Krause
Room: Grand West

Scheduled Time: 9:05 AM
Duration: 25 Minutes
What to Do with Mistakes in the PDB: Resolving the Active Site of PYCR1. John Tanner.

Scheduled Time: 9:30 AM
Duration: 30 Minutes
Ligand Validation for the Protein Data Bank. Stephen Burley.

Scheduled Time: 10:35 AM
Duration: 30 Minutes
Ensuring accurate modeling in its electron density of a ligand bound to a therapeutic target in a high throughput environment: a review of best practices. Thierry Fischmann.

Scheduled Time: 11:05 AM
Duration: 30 Minutes
Software Tools in Coot and CCP4 for Dictionaries and Validation of Ligands. Paul Emsley.

Scheduled Time: 11:35 AM
Duration: 25 Minutes
Polder maps: Improving OMIT maps for ligand building and validation. Dorothée Liebschner.

3.1.3 Theoretical and Computational Crystallography - Present and Future Opportunities at the Structural Interface of Experiment and Theory
Chairs: Branton Campbell & Wenhao Sun
Room: Provincial North
MONDAY | JULY 23

Scheduled Time: 9:00 AM  
Duration: 30 Minutes  
Insightful crystal-structure classification using deep learning. Angelo Ziletti, Matthias Scheffler.

Scheduled Time: 9:30 AM  
Duration: 30 Minutes  

Scheduled Time: 10:30 AM  
Duration: 30 Minutes  

Scheduled Time: 11:00 AM  
Duration: 20 Minutes  

Scheduled Time: 11:20 AM  
Duration: 20 Minutes  
Adventures in diffraction - from atomic form factors to resolution of defects. Peter Khalifah.

Scheduled Time: 11:40 AM  
Duration: 20 Minutes  

3.1.4 Next Generation Sources/SAS @ New Sources  
Chairs: Marjolein Thunnissen & Ray Sierra  
Room: Grand East

Scheduled Time: 9:25 AM  
Duration: 25 Minutes  

Scheduled Time: 9:45 AM  
Duration: 20 Minutes  
The rise of BioSAXS at the ESRF: BM29 Beamline for SAXS on Proteins in Solution. Petra Pernot, Martha Brennich.

Scheduled Time: 10:35 AM  
Duration: 20 Minutes  

Scheduled Time: 10:55 AM  
Duration: 20 Minutes  

Scheduled Time: 11:15 AM  
Duration: 20 Minutes  

3.1.5 Crystallography at Extreme Conditions  
Chairs: Camelia Stan & Cristine Beavers  
Room: Provincial South

Scheduled Time: 9:00 AM  
Duration: 15 Minutes  
In-situ Synchrotron High Pressure Laser Heating Experiments. Emma Ehrenreich-Petersen, Camilla Hjort Kronbo.

Scheduled Time: 9:15 AM  
Duration: 15 Minutes  

Scheduled Time: 9:40 AM  
Duration: 20 Minutes  
Are we prepared for “Big Data” in high pressure sciences?. Clemens Prescher.
Scheduled Time: 10:30 AM
Duration: 20 Minutes

Scheduled Time: 10:50 AM
Duration: 15 Minutes
New Non-Traditional Experimental Techniques to Study Materials at High Pressures. Matthew Whitaker, Melinda Rucks.

Scheduled Time: 11:05 AM
Duration: 15 Minutes
High-Pressure and High Temperature Behavior of Datolite. Carla Slebodnick, Jing Zhao.

Scheduled Time: 11:20 AM
Duration: 15 Minutes
Strain-rate and temperature effects on kinetics and phase transitions for albite and olivine. Melissa Sims, Melinda Rucks.

Scheduled Time: 11:35 AM
Duration: 15 Minutes
Investigation of Tissintite Formation and Its Implications for Impact Studies. Melinda Rucks, Matthew Whitaker.

Scheduled Time: 11:50 AM
Duration: 10 Minutes

3.2.1 Structural Biology of Inherited Metabolic Disorders: Personalized Biochemistry and Biophysics
Chairs: Lesa Beamer & Jack Tanner
Room: Grand Centre

Scheduled Time: 1:30 PM
Duration: 40 Minutes
From Structural Biology to Small Molecule Therapy for Inborn Errors of Metabolism. Wyatt Yue.

Scheduled Time: 2:10 PM
Duration: 15 Minutes
Molecular mechanisms of enzyme dysfunction in PGM1 deficiency, an inherited metabolic disease. Kyle Stiers.

Scheduled Time: 2:25 PM
Duration: 15 Minutes
Structure Analysis of Human Prolidase Mutations gives insight into the Prolidase Deficiency disease mechanisms. Piotr Wilk.

Scheduled Time: 2:40 PM
Duration: 20 Minutes
 Disequilibrium of porphobilinogen synthase assemblies accounts for ALAD porphyria. Eileen Jaffe.

Scheduled Time: 3:30 PM
Duration: 40 Minutes
Structural and energetic insights into CF-causing mutations in CFTR. Julie Forman-Kay, Robert Vernon.

Scheduled Time: 4:10 PM
Duration: 15 Minutes
Single-residue variants of phenylalanine hydroxylase help to observe multiple structural isoforms that comprise the structural equilibrium. Emilia C Arturo, Michael Riis Hansen.

Scheduled Time: 4:25 PM
Duration: 15 Minutes
Pyruvate dehydrogenase complex deficiency disease is connected to regulatory loop disorder in the alphaV138M variant of human pyruvate dehydrogenase. Matthew Whitley, Palaniappa Arjunan.
Scheduled Time: 4:40 PM  
Duration: 15 Minutes  
Leveraging Protein Structure and Dynamics for Variant Interpretation in Coding Regions. Mark Gerstein, Declan Clarke.

3.2.2 Crystallization on the International Space Station  
Chairs: Ken Savin & Marc Giulianotti  
Room: Grand West

Scheduled Time: 1:30 PM  
Duration: 15 Minutes  
CASIS Perspective on the Use of the International Space Station National Laboratory for Crystallization Experiments. Marc Giulianotti, Ken Savin.

Scheduled Time: 1:45 PM  
Duration: 20 Minutes  

Scheduled Time: 2:05 PM  
Duration: 20 Minutes  
Microgravity Biologics Crystallization Processes. Paul Reichert.

Scheduled Time: 2:25 PM  
Duration: 20 Minutes  
Inorganic salt crystallizations by thermal gradient technique. Ilia Guzei, April Spinale.

Scheduled Time: 3:40 PM  
Duration: 20 Minutes  
Measure and Might of the MiTeGen In Situ-1™ Crystallization Plate for Microgravity Protein Crystal Growth. Kristofer Gonzalez-DeWhitt.

Scheduled Time: 4:00 PM  
Duration: 20 Minutes  

Scheduled Time: 4:20 PM  
Duration: 20 Minutes  

Scheduled Time: 4:40 PM  
Duration: 20 Minutes  
A simple crystallization device for growing large protein crystals. Hiroaki Tanaka, Sachiko Takahashi.

3.2.3 Theoretical and Computational Crystallography - Present and Future Opportunities at the Structural Interface of Experiment and Theory  
Chairs: Peter Khalifah & Wenhao Sun  
Room: Provincial North

Scheduled Time: 1:30 PM  
Duration: 30 Minutes  
Machine Learning and Materials Discovery*. Gus Hart.

Scheduled Time: 2:00 PM  
Duration: 20 Minutes  
Some theoretical and computational aspects of nanocluster structure solution. Simon Billinge.

Scheduled Time: 2:40 PM  
Duration: 20 Minutes  

Scheduled Time: 3:30 PM  
Duration: 30 Minutes  
Crystal structure prediction in novel nitrides: The roles of metastability and disorder. Stephan Lany.

Scheduled Time: 4:00 PM  
Duration: 15 Minutes  
3.2.4 Scattering Strategies in Biomembrane Research

Chairs: Frederick Heberle, Drew Marquardt & Maikel Rheinstadter
Room: Grand East

Scheduled Time: 1:30 PM
Duration: 40 Minutes
From collective fluctuations to the mechanical properties of model biological membranes using neutron spin echo spectroscopy. Michihiro Nagao, Elizabeth Kelley.

Scheduled Time: 2:10 PM
Duration: 15 Minutes

Scheduled Time: 2:25 PM
Duration: 20 Minutes
Determining the transbilayer structure of asymmetric bilayer membranes using small-angle scattering. Frederick Heberle.

3.2.5 Mineralogical Crystallography

Chairs: Nichole Valdez & Aaron Celestain
Room: Provincial South

Scheduled Time: 1:30 PM
Duration: 30 Minutes
The intriguing crystal structure of the rhabdophane mineral LnPO4.nH2O. Adel MESBAH, Nicolas Clavier.

Scheduled Time: 2:00 PM
Duration: 20 Minutes
Scheduled Time: 2:20 PM
Duration: 20 Minutes

Scheduled Time: 2:40 PM
Duration: 20 Minutes
High-Pressure Structural and Equation of State Study of Xenotime. Nancy Ross, Jing Zhao.

Scheduled Time: 3:30 PM
Duration: 30 Minutes
Data-mined ion substitutions in crystals: Reassessment of Goldschmidt’s rules of ion substitution. Olivier Gagné, Robert M. Hazen.

Scheduled Time: 4:00 PM
Duration: 20 Minutes

Scheduled Time: 4:20 PM
Duration: 20 Minutes
Understanding the formation of polytypism in natural moissanite with Laue microdiffraction. Camelia Stan, Earl O’Bannon.

Scheduled Time: 4:40 PM
Duration: 20 Minutes
Stacking faulted crystal structures can require correlation coefficients in their modelling. Alan David Rae.

3.3.1 Diversity & Inclusivity
Chairs: Bernard Santarsiero
Room: Provincial North

Scheduled Time: 6:35 PM
Duration: 40 Minutes
NSF Improving Undergraduate STEM Education (IUSE) for Hispanic-Serving Institutions (HSI). Talitha Washington.
PL3 Etter Early Career Award to Jason McLellan
Lisa J. Keefe, Presiding
Room: Grand Centre

Scheduled Time: 8:00 AM
Using X-ray Crystallography to Fight Back Against Pneumoviruses.
Jason McLellan.

4.1.1 Structural Biology of Pathogens: Cellular Interactions, Drug Resistance, and Immune Responses
Chairs: B.V.V. Prasad, Jean-Philippe Julien & Michael Becker
Room: Grand Centre

Scheduled Time: 9:00 AM
Structural and Mechanistic Basis for Drug Resistance Mutations in Altering the Specificity of CTX-M beta-lactamas-
es. Timothy Palzkill.

Scheduled Time: 9:30 AM

Scheduled Time: 9:45 AM
Structural basis of glycan specificity in human rotaviruses. Liya Hu.

Scheduled Time: 10:30 AM
Microbial biofilms: Molecular mechanisms to potential therapeutics. Lynne Howell.

Scheduled Time: 11:00 AM
Structural Insight Into a Heme Relay from Human Hemoglobin to SbnI, a Regulator of Siderophore Biosynthesis in S. aureus. Michael Murphy, Anson Chan.

Scheduled Time: 11:15 AM
Duration: 30 Minutes
Structural Basis for Antagonism of Bacterial LPS Transport. Christopher Koth, Hoangdung Ho.

Scheduled Time: 11:45 AM
Duration: 15 Minutes
Structure of a Lipid-bound Viral Membrane Assembly Protein Reveals a Novel Modality for Interacting with Lipid Bilayer. Shuxia Peng.

4.1.2 Minding the Gap: MX to XFEL / Open Science
Chairs: Jenifer Wierman & Ana Gonzalez
Room: Provincial North

Scheduled Time: 9:00 AM
Duration: 20 Minutes
Sample Manipulation and Data Assembly for Robust Microcrystal Synchrotron Crystallography. Qun Liu.

Scheduled Time: 9:20 AM
Duration: 20 Minutes
Metalloprotein Oxidation States Spatially Resolved by Anomalous Dispersion Crystallography. Nicholas Sauter, James Holton.

Scheduled Time: 9:40 AM
Duration: 25 Minutes
What dose DOES a micro-crystal really absorb?. Elspeth Garman, Charles Bury.

Scheduled Time: 10:35 AM
Duration: 25 Minutes
New Opportunities for Structural Biology Research at LCLS and SSRL. Aina Cohen.

Scheduled Time: 11:00 AM
Duration: 20 Minutes
A High-Throughput Serial Crystallography Beamline at CHESS. Doletha Szebenyi, Aaron Finke.
Scheduled Time: 11:20 AM
Duration: 20 Minutes
Fixed-targets Serial crystallography at SPring-8 and SACLA. MASAKI YAMAMOTO, Kazuya Hasegawa.

Scheduled Time: 11:40 AM
Duration: 20 Minutes
Improving Unit-Cell Distance Algorithms for Clustering MX images. Herbert J. Bernstein, Lawrence C. Andrews.

4.1.3 Cool Structures
Chairs: Shao-Liang Zheng & SuYin Grass Wang
Room: Grand West
Scheduled Time: 9:00 AM
Duration: 20 Minutes
Packing polymorphs and high Z' structures obtained by different crystallization conditions. Tatiana Timofeeva.

Scheduled Time: 9:20 AM
Duration: 20 Minutes
Mixed-Valence Copper Cyanide Polymers – Successes, Surprises and Disappointments. Peter Corfield, Joseph Dayrit.

Scheduled Time: 9:40 AM
Duration: 20 Minutes
Exploring the coordination chemistry of imidoyl amidine ligands with first row transition metals. Raúl Castañeda, Bulat Gabidullin.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
The missing link: first successful structural analysis of 2-ethylimidazole, a ZIF linker. Stacey Smith.

Scheduled Time: 10:50 AM
Duration: 20 Minutes
Structure of a 1.5-MDa bacterial adhesin reveals its role in the mixed-species biofilm formation with diatoms on ice. Shuaiqi Guo, Ilja Voets.

Scheduled Time: 11:10 AM
Duration: 20 Minutes
Crystal structures of the RLPH2 protein phosphatase from Arabidopsis thaliana reveal a novel mechanism for recognizing dually phosphorylated substrates. Kenneth Ng, Anne-Marie Labandera.

Scheduled Time: 11:30 AM
Duration: 15 Minutes

4.1.4 Application of SAS to Complex Mixtures
Chairs: Thomas Weiss & Nigel Kirby
Room: Grand East
Scheduled Time: 9:00 AM
Duration: 30 Minutes
Better Data with SEC-SAXS. Thomas Wiess, Tsutomu Matsui.

Scheduled Time: 9:30 AM
Duration: 30 Minutes
Characterizing solution dynamics of highly flexible enzymes. Maxwell Watkins, Hao Li.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
Alpha-catenin structure in solution and in complex with F-actin as revealed by small angle X-ray and neutron scattering study. Zimei Bu.
Scheduled Time: 10:50 AM
Duration: 20 Minutes
SEC-SAXS studies of double-stranded RNAs from trypanosome RNA editing. Blaine Mooers, Tsutomu Matsui.

Scheduled Time: 11:10 AM
Duration: 20 Minutes
Coflow SEC-SAXS at High Flux. Nigel Kirby, Tim Ryan.

Scheduled Time: 11:30 AM
Duration: 30 Minutes

4.1.5 Operando & In-Situ Studies
Chairs: Wenqian Xu & Sanjit Ghose
Room: Provincial South

Scheduled Time: 9:00 AM
Duration: 20 Minutes
Observing Crystallization Pathways In situ. Michael Toney.

Scheduled Time: 9:20 AM
Duration: 20 Minutes

Scheduled Time: 9:40 AM
Duration: 20 Minutes
Real time data collection in multidimensional diffraction and parameter spaces. Xiaoping Wang.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
Measurement and Analysis of in operando / situ Lithium-Ion battery data on a XRPD laboratory diffractometer. Thomas Degen, Milen Gateshki.

Scheduled Time: 10:50 AM
Duration: 20 Minutes
Probing the Electrode-Electrolyte Interface with In-Operando Neutron Scattering. Craig Bridges, Charl Jaffa.

Scheduled Time: 11:10 AM
Duration: 20 Minutes
Understanding the role of chemical inhibitors to the deposition of wax from crude oil. Thomas Fitzgibbons, Larisa Reyes.

Scheduled Time: 11:30 AM
Duration: 15 Minutes
In-situ visualization of loading-dependent water effects in a stable metal-organic framework. Nicholas Burch.

Scheduled Time: 11:45 AM
Duration: 15 Minutes
Search for new phases using in-situ reduction technique in the K-Sn-O System. Rebecca McAuliffe, Daniel Shoemaker.

4.2.1 Regulation of Protein Function by Shape Shifting
Chairs: Erica O Saphire, Emilia C Arturo & Eileen K. Jaffe
Room: Grand Centre

Scheduled Time: 1:40 PM
Duration: 15 Minutes

Scheduled Time: 1:55 PM
Duration: 20 Minutes

Scheduled Time: 2:15 PM
Duration: 20 Minutes
Conformational changes in the peptidoglycan synthase activator LpoA are likely important for maintaining a viable cell wall in Gram-negative bacteria. Mark Saper & Karthik Sathiyamoorthy.
Another piece of the jigsaw: a new signaling axis defined by shape-specific RNR- hexamers. Yimon Aye.

Scheduled Time: 2:35 PM
Duration: 25 Minutes


Scheduled Time: 3:30 PM
Duration: 20 Minutes

Hierarchical structures of HIV Integrase: Drug-induced Aggregates of HIV Integrase are Weak Gels. Kushol Gupta.

Scheduled Time: 4:15 PM
Duration: 25 Minutes

Regulation of Morpheein Behavior in B. cenocepacia HMG-CoA Reductase. Jeff Watson & Chad Hicks.

Scheduled Time: 4:40 PM
Duration: 20 Minutes


4.2.2 General Interest - 2
Chairs: Michael Takase & Laura Van Staaldruinen
Room: Grand East

Scheduled Time: 1:30 PM
Duration: 15 Minutes

Antibody Fab Fragments and their Crystal Organization. Travis Gallagher & Loannis Karageorgos.

Scheduled Time: 1:45 PM
Duration: 15 Minutes

Protein Tag Mediated Fusion Protein Crystallization. Tengchuan Jin.

Scheduled Time: 2:00 PM
Duration: 15 Minutes

New structural insight into HMG-CoA reductase mechanism and cofactor specificity. Yan Kung & Bradley Miller.

Scheduled Time: 2:15 PM
Duration: 15 Minutes


Scheduled Time: 2:30 PM
Duration: 15 Minutes

Structural Metamorphosis of the Fe(III) Gallate – a Historical Iron Gall Ink. Peter Y. Zavalij.

Scheduled Time: 2:45 PM
Duration: 15 Minutes

Structural Chemistry of Azulenes. Nick Gerasimchuk & Mikhail Barybin.

Scheduled Time: 3:30 PM
Duration: 15 Minutes


Scheduled Time: 3:45 PM
Duration: 15 Minutes

Crystal structure of a 6.5 MDa bacterial microcompartment shell. Markus Sutter.

Scheduled Time: 4:00 PM
Duration: 15 Minutes

Analysis of crystallographic structures and DFT calculations reveal a new structural arrangement in proteins involving lysine NH3+ group and carbonyl. Nikolai R. Skrynnikov & Sergei A. Izmailov.

Scheduled Time: 4:15 PM
Duration: 15 Minutes

Metalloprotein Plasticity: Cautionary Tales. Nicholas Schnicker.
Scheduled Time: 4:30 PM  
Duration: 15 Minutes  

Scheduled Time: 4:45 PM  
Duration: 15 Minutes  
Charge Density: The Devil is in the Details. Bruce C. Noll & Holger Ott.

4.2.3 Engaging Undergrads with Crystallographic Research  
Chairs: Joe Tanski & Rachel Powers  
Room: Provincial North

Scheduled Time: 1:35 PM  
Duration: 20 Minutes  

Scheduled Time: 1:55 PM  
Duration: 20 Minutes  

Scheduled Time: 2:15 PM  
Duration: 20 Minutes  

Scheduled Time: 2:35 PM  
Duration: 25 Minutes  

Scheduled Time: 3:30 PM  
Duration: 20 Minutes  
Establishing a New Protein X-ray Crystallography Research Group at a PUI. Krystle McLaughlin.

Scheduled Time: 3:50 PM  
Duration: 20 Minutes  

Scheduled Time: 4:10 PM  
Duration: 20 Minutes  

Scheduled Time: 4:30 PM  
Duration: 25 Minutes  
A Scaffolded Approach to the Integration of Crystallography in Undergraduate Curriculum and Research. Louise Dawe.

4.2.4 Powder Diffraction of Industrial and Pharmaceutical Materials  
Chairs: Silvina Pagola & Jim Kadak  
Room: Grand West

Scheduled Time: 1:30 PM  
Duration: 22 Minutes  
The Powder Diffraction Mail-In Program at the Canadian Light Source: A Useful Tool for Industrial and Basic Research. Joel Reid.

Scheduled Time: 1:52 PM  
Duration: 23 Minutes  
Crystal Structures of Large-Volume Commercial Pharmaceuticals. Jim Kaduk.

Scheduled Time: 2:15 PM  
Duration: 22 Minutes  
Incorporation of Pharmaceutical API’s into the PDF® Databases. Amy Gindhart & Tom Blanton.

Scheduled Time: 2:37 PM  
Duration: 23 Minutes  
Scheduled Time: 3:30 PM  
Duration: 22 Minutes  
WinPSSP: a free-distribution software for the crystal structure determination of organics from powders. Silvina Pagola.

Scheduled Time: 3:52 PM  
Duration: 23 Minutes  

Scheduled Time: 4:15 PM  
Duration: 22 Minutes  
A New Malaria Pigment Structural Motif and Potential Drug Target. Peter Stephens.

Scheduled Time: 4:37 PM  
Duration: 23 Minutes  
Improved crystal structure solution from powder diffraction data by the use of conformational information. Elena Kabova.

Scheduled Time: 1:30 PM  
Duration: 15 Minutes  

Scheduled Time: 1:45 PM  
Duration: 15 Minutes  

Scheduled Time: 2:00 PM  
Duration: 20 Minutes  
Discovery of the Third Ambient Aspirin Polymorph. Chunhua Tony Hu & Alexander G. Shtukenberg.

Scheduled Time: 2:20 PM  
Duration: 20 Minutes  
Synthesis of a family of Pt-Ag clusters: Ligands, solvents, unit cells and crystal quality. Milagros Tomás & Irene Ara.

Scheduled Time: 2:40 PM  
Duration: 20 Minutes  
From Crystal Structures to Rotational Excitations of Bound H2 by Computer Simulations. Juergen Eckert.

Scheduled Time: 3:30 PM  
Duration: 15 Minutes  

Scheduled Time: 3:45 PM  
Duration: 15 Minutes  

Scheduled Time: 4:00 PM  
Duration: 20 Minutes  
Enantiomeric resolution of helicochiral paddlewheel complexes and their infrared, Raman, UV-vis and X-ray optical activity. Elizabeth Hillard & Thierry Buffeteau.

Scheduled Time: 4:20 PM  
Duration: 20 Minutes  
Before and After: Can we predict and/or understand an observed twin law using extant tools and a look at plausible composition planes?. Bruce Foxman & Victor Young.

Scheduled Time: 4:40 PM  
Duration: 20 Minutes  
TUESDAY | JULY 24

ANNUAL AWARDS BANQUET

6:30 PM - 7:30 PM Cash Bar [Grand Foyer]
7:30 PM Banquet Doors Open [Grand Centre]
After dinner entertainment by the Stringhoppers

WEDNESDAY | JULY 25

2019
Planning Meeting

9:00 AM - 11:00 AM
[Wentworth Room]

SAVE THE DATES!

2019
Cincinnati/northern KY
Saturday, July 20, 2019 - Wednesday, July 24, 2019

2020
San Diego, California
Friday, July 31, 2010 - Friday, August 7, 2020
ETTER STUDENT AWARDS

2018 Margaret C. Etter Student Lecturer Awards

Each Scientific Interest Group (SIG) has the opportunity to select one student to receive an award and to present a lecture. Selections are based upon submitted abstracts and are independent of whether the student originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected receive a monetary award of $250 and a certificate to be presented at the beginning of their lecture.

Congratulations to the 2018 Etter Lecturers:

Raúl Castañeda .................. 4.1.3 Exploring the coordination chemistry of imidoyl amidine ligands with first row transition metals

William Thomas .................. 4.2.1 A Novel Form of Allosteric Regulation in Bacillus subtilis Ribonucleotide Reductase Revealed by SAXS and Cryo-Electron Microscopy

Maxwell Day .................... 3.2.5 A structure hierarchy for chain-, ribbon- and tube-silicate minerals: a bond topological approach

Jessica L. Thomaston ............ 3.1.1 Structural characterization of adamantane-resistant mutants of the influenza M2 proton channel

David Moreau .................... 2.2.3 Ice formation in protein crystals: effects of nan confinement

Luiza Germann ................... 4.2.4 Real-time monitoring of mechanochemical formation of pharmaceutical cocrystals using synchrotron X-ray diffraction

Juby Varghese ................. 2.1.5 Metal-Organic Frameworks as Platforms for the Nanostructuration of Single Molecule Magnets: New Insights from HRTEM

Stephanie Gnewuch ............ 1.1.4 A Comparison of the Magnetic Structures of Candidate Ferrotoroidic Olivine Materials

Matrew Logan ................... 2.1.5 Systematic Isoreticular Expansion of Titanium Metal-Organic Frameworks

Seth Cory ......................... 4.1.3 Structure of the human Fe-S cluster assembly sub-complex: implications in Friedreich’s ataxia and primary metabolism

Maxwell Watkins ............... 4.1.4 Characterizing solution dynamics of highly flexible enzymes

Cara Vennari .................... 3.1.5 High-Pressure/Temperature Behavior of the Alkali/Calcium Carbonate Shortite (Na2Ca2(CO3)3): Implications for Carbon Sequestration in the Deep Earth

Emilia C. Arturo ................ 3.2.1 Single-residue variants of phenylalanine hydroxylase help to observe multiple structural isoforms that comprise the structural equilibrium
Pauling Poster Prizes
The Pauling Poster Prizes were established by the ACA to honor Linus Pauling and are supported by member donations. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each meeting, the five best graduate or undergraduate poster presentations receive Pauling awards. Each award consists of $250, a complimentary banquet ticket, and a copy of a Linus Pauling book. An additional Pauling Prize sponsored by the Canadian Div. of the ACA and the Canadian National Committee, will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory.

IUCr Poster Prize
The IUCr Executive Committee is pleased to continue a series of IUCr awards presented at meetings of the regional affiliates and national crystallographic associations. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of International Tables or other IUCr publication.

Journal on Structural Dynamics Poster Prize
A prize of $250 is given for excellence in research on structural determination and dynamics of systems, enabled by emerging new instruments (e.g., XFELs, electron sources, etc.) and new experimental and theoretical methodologies and is open to students (graduate and undergraduate) and post-docs.

RCSB Protein Data Bank Poster Prize
This prize recognizes a student poster presentation involving macromolecular crystallography. The award will be 2 educational books that will be mailed to the winner after the meeting. An announcement will appear on the RCSB PDB website and newsletter.

CrystEngComm Poster Prize
CrystEngComm (published by the Royal Society of Chemistry) is very pleased to sponsor a prize to be awarded to the best graduate or undergraduate poster presentation in the area of crystal engineering/supramolecular chemistry. The winner will receive an RSC book voucher and an announcement will be posted on the CrystEngComm website (www.rsc.org/Publishing/Journals/CE/about.asp) shortly after the conclusion of the meeting.

Oxford Cryosystems Low Temperature Poster Prize
This prize is open to all participants and is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc.

Journal of Chemical Crystallography Poster Prize
The best graduate or undergraduate poster presentation in the area of chemical crystallography or small molecule structure determination and analysis is sponsored by Springer’s Journal of Chemical Crystallography. The winner will receive their personal choice of books from Springer’s extensive portfolio of titles.

Taylor & Francis Biomolecular Crystallography Poster Prize
This prize is open to all participants and is awarded to the best poster describing a successful application of a non-routine or computationally challenging structure solution and refinement technique in biomolecular crystallography. The winner will receive Bernhard Rupp’s book Biomolecular Crystallography donated by the Taylor & Francis Group and will be announced at the banquet.
POSTERS

POSTER HANGING INSTRUCTIONS
All posters should be displayed from 10:30 am on Saturday, July 21, until 7:30 pm on Monday, July 23. Please be present at your poster from 5:30 - 7:30 pm on the day to which you are assigned. Posters beginning with SA present on Saturday. Posters beginning with SU present on Sunday. Poster beginning with MO present on Monday.

SA1

SA2

SA3
Use of polysterism analysis to probe the conformational landscape and residue networks within an a-D-phosphohexomutase. Lesa Beamer.

SA4
A compact, low power infrared tube furnace for in-situ and in-operando X-ray powder diffraction. Christine Beavers.

SA5
Structure of a Green Fluorescent Protein Biosensor – Implications for FRET. Stefan Becker.

SA6

SA7

SA8

SA9
Algebraic search for cooperative-rotational rigid-unit modes. Branton Campbell.

SA10
Discovering Inhibitors of Rumen Methanogens Using High-Throughput X-ray Crystallography and Enzyme Screening Techniques. Vince Carbone.

SA11
Ligand-modulated ring expansion. Veronica Carta.

SA12
Structural Diversity of Mercury (II) Complexes Derived from Substituted Pyrazoles. Indranil Chakraborty.

SA13
Tetrameric structure of the flagellar cap protein FlID from Serratia marcescens. Soyeon Cho.

SA15
Characterization of the Dual Function of ATXR5 PIP motif in PCNA and Nucleosome Binding. Hossein Davarinejad.

SA16
The small-angle X-Ray Scattering core facility of center for cancer research of National Cancer Institute. Lixin Fan.
Using topology of molecular solvation to enhance biomolecular structural refinement. George Giambasu.


Pyridine Complexes of Some First Row Transition Metals. James Golen.

Resolution of an antifungal compound through co-crystallisation. Michael Guillot.


Effects of PKA and CaMKII Phosphorylation on the Ryanodine Receptor Phosphorylation Domain. Omid Haji-Ghassemi.

Analysis of crystal size and wavelength dependence using the deep UV laser processing crystals. Ayaka Harada.

Structure Based Drug Design of Clinical Compound MK-8353, a Novel inhibitor of ERK. Alan Hruza.

Pseudo-Complementary Base-Pairing Involving Sulfur as a Robust Design Element in Crystal Engineering. Wilhelm Maximilian Hützler.


Tracking active-site solvents in human carbonic anhydrase II. Jin Kyun Kim.

Nucleation of protein crystals using surface energy modified substrate. Tiffany Kinnibrough.


Two Energetic Cocrystals of TNT/cyclohexane and picric acid/triethylamine. Yan Li.

Sample concentration and buffer exchange utilizing a miniaturized tangential flow filtration (TFF) system. Baker Logan.

Deciphering the role of the Bateman domain in IMPDHs. Hélène Munier-Lehmann.

SA37

SA38

SA39
The time machine: structure-based elucidation of timekeeping mechanisms by the cyanobacterial circadian clock. Carrie Partch.

SA41
Structural insights into the mechanism of ubiquitination by the linear ubiquitin chain assembly complex (LUBAC). Simin Rahighi.

SA42
Structure-guided engineering fine-tunes pharmacokinetics, tolerability, and anti-tumor profile of anti-frizzled antibody. Swetha Raman.

SA43
In-Situ Characterization of the Synthesis of Ca12Al14O33 Under Non-Ambient Atmospheres. Claudia Rawn.

SA44

SA45
Crystallographic exploration of flexibility in an allosteric enzyme. David Schuller.

SA46
The Role of Tetramethylethylenediamine (TMEDA) in Iron Catalyzed Cross-Coupling Reactions. Jeffrey Sears.

SA48
Acidochromic Spiropyran-Merocyanine stabilisation in the solid state. Vanessa Kristina Seiler.

SA49

SA50
Crystal Structure of a Rationally Designed Six-Fold Symmetric DNA Scaffold for the Precise Organization of Biomolecules. Chad Simmons.

SA51
Chiral Segregation of Space by Anionic Assemblies found in Tartramide-based Spiroborate Salts. Aristyo Soecipto.

SA52

SA53
A practical method for an efficient and optimal production of selenomethionine-labeled recombinant protein complexes in the insect cells. Yuichiro Takagi.

SA55

SA56
Structure of HIV-1 TAR in Complex with a Lab-Evolved Protein Provides Insight into RNA Recognition and Synthesis of a Constrained Peptide that Impairs Transcription. Joseph E Wedekind.
SA57
Defining the dynamics behind Ryanodine Receptor modulation by small molecules. Kellie Woll.

SA58
Do diverse antifreeze protein structures bind ice by the same mechanism?. Qilu Ye.

SA59
Structural studies of arginine decarboxylase in Helicobacter pylori. Huawei Zhang.

SU60
Purification and characterization of Band 3 complexes from human erythrocyte membranes. Yazan Abbas.

SU61

SU62
Structural insights into biofilm polysaccharide de-N-acetylation in the fungus Aspergillus fumigatus. Natalie Bamford.

SU63
Investigation of a Novel Slam Dependent Heme Acquisition System in the Bacterial Pathogen Acinetobacter baumannii. Tom Bateman.

SU64
Crystallisation and Initial Characterization of the periplasmic domain of TraG, the Conjugative Entry Exclusion Protein from the F-plasmid. Nicholas Braganholo.

SU65
Novel protease inhibitors markedly adapting to the structural plasticity of HIV-1 protease exert extreme potency with high genetic barrier. Haydar Bulut.

SU66

SU67
Structural Analysis of Multiple Lab-Evolved Proteins that Bind HIV-1 TAR RNA with NanoMolar Affinity. Sai Shashank Chavali.

SU68
Structural Determinants for the Activation of Soluble Guanylyl Cyclase. Kenneth Childers.

SU69
Structural and Functional Analysis of Yeast Shu Complex. Sam Chu.

SU70
Structural analysis on Salmonella effector SseK3-UDP complex. Ivy Chung.

SU71
Structure and Function of Terfesstatin Biosynthesis Proteins TerB and TerC. Jonathan Clinger.

SU72
Structural characterization of a novel amino acid decarboxylase. Raquel Sofia Correia Cordeiro.

SU73
Structural Changes and Control on Conjugation of Glutathione with Chalcones and their Quinolinone Analogues. Jean Custodio.

SU74
The residues in the hydrophobic core of Staphylococcus aureus Fatty acid Kinase B1 determine fatty acid specificity. Maxime Cuypers.
SU75
Crystallization of Novel Polyglycine Hydrolases from two fungal families: Epicoccum sorghi and Fusarium solani. Nicole Fraser.

SU76

SU77
Role of AlgL in Pseudomonas aeruginosa alginate biosynthesis. Andreea Gheorghita.

SU78
Mechanism of Rad5-mediated DNA rearrangement in error-free template switching. Melissa Gildenberg.

SU79
Evidence for Breathing of a Class I Fusion Protein at the Cell Surface. Morgan Gilman.

SU80
A Database Conundrum - MD, SAXS and NMR disorder data. Garrett Ginell.

SU81
Structural insights into the dimeric human PNPase revealing why the disease-linked mutants exhibit lower RNA import and degradation activities. Bagher Golzarroshan.

SU82
First experimental visualization of the gaseous product CO2 in the active site of ODCase supports substrate strain as an integral part of the catalytic mechanism. Ondrej Halgas.

SU83
Supramolecular Effects to Explain a Nonstatistical Disorder. Joseph Haller.

SU84
2-Hydroxy-3,5-dinitrobenzoate: A Novel μ2-Bridging Ligand. Jeffrey Haller.

SU85
Structural Studies of Human ATP-Specific Succinyl-CoA Synthetase. Ji Huang.

SU86
Structural basis for human DNA polymerase kappa to bypass cisplatin intrastrand cross-link (Pt-GG) lesion as an efficient and accurate extender. Vikash Jha.

SU87
EM studies of cytochrome bc1 to elucidate inhibitor binding. Rachel Johnson.

SU88
Structure-guided fusion-protein designs using Bacillus flagellin as a vaccine adjuvant. Meong il Kim.

SU89
Structural insight into degradation mechanism of N-end rule substrates by p62/SQSTM1 selective autophagy adaptor. Do Hoon Kwon.

SU90

SU91

SU92
Substrate specificity of N-methyltransferases in benzylisoquinoline alkaloid metabolism. Dean Lang.
SU93 Structural and Functional Analysis of a PadR-like Transcription Factor From Bacteroides fragilis. Choongdeok Lee.

SU94 Pgp2 is an LD-Carboxypeptidase that Determines the Helical Cell Shape of Campylobacter jejuni. Chang Sheng-Huei Lin.

SU95 Cancer-associated mutations of the pre-mRNA splicing factor U2AF2 alter splice site signal recognition. Debanjana Maji.

SU97 Effect of pH on Fe-O2 bond in the oxygen reactive hemoglobins of L.pectinata by X-ray Crystallography. Darya Marchany-Rivera.

SU98 The molecular mechanism of the type IVa pilus motor. Matthew McCallum.


SU100 Optimizing small molecules as a chemical tool to control DNA Repair enzymes using X-ray crystallography and computational techniques. Davide Moiani.

SU101 Structural investigation of the oligomeric domain of the psychiatric risk protein DISC1. Anand Nambisan.


SU103 Expression and characterization of Lactase Phlorizin Hydrolase region III. Nardo Nava.

SU104 Determining the mechanism of LINE-1 ribonucleoprotein particle assembly and inhibition by nucleoside reverse transcriptase inhibitors. Jocelyn Newton.


SU106 Structural Determinants of LTA4H Aminopeptidase Activation. Schroeder Noble.

SU107 Crystal structure of an As(III) S-adenosylmethionine methyltransferase with both bound ligand and product demonstrates a conformational change in the N-terminal domain during catalysis. Charles Packianathan.


SU109 Overexpression, purification of GSK3 and it’s interaction with an inhibitory fragment of the psychiatric risk protein DISC1. Narsimha Pujari.

SU110 Disorder, disulfides and domain-swaps in an oxidized octamer of a gS-crystallin. Vatsala Sagar.

SU111 Neutron structure and mutagenic analysis of human ABO bloodgroup glycosyltransferases support an orthogonal associative mechanism of stereospecificity. Brock Schuman.
SU112
Using the 3-D structures of the viral proteinases of Porcine Epidemic Diarrhoea Virus (PEDV) to design anti-PEDV drugs. Tooba Naz Shamsi.

SU113
Structural and Functional Studies of E.coli Guanine Deaminase. Roger Shek.

SU114
Mechanistic underpinnings of allostery, catalysis and domain synchronization in an ammonia tunneling enzyme. Santosh Shivakumaraswamy.

SU115

SU116
Structural Basis of Conserved Flagellin-mediated TLR5 Stimulation. Wanseok Song.

SU117
DNA Damage Repair - Investigating the Conformations of DNA Ligase and PCNA. Aleksandr Sverzhinsky.

SU118
Crystallization and structural studies of an aldo-keto reductase from opium poppy. Miguel Torres.

SU119
Conformational flexibility of pore loop-1 gives insights into substrate translocation by AAA+ protease FtsH. Matthias Uthoff.

SU120
Diverse ligand-binding domain combinations at the distal end of bacterial RTX adhesins are postal codes for biofilm formation. Tyler Vance.

SU121
Molecular Mechanisms of AlPL1 and its TPR domain in Leber congenital amaurosis 4 (LCA4) a severe form of childhood blindness. Ravi Prakash Yadav.

SU122

SU123
Cfp1/Cps40 stabilizes MLL complex formation through multi-valent interactions. Yidai Yang.

SU124
SPOP Oligomerization Drives the Assembly of Multivalent Cullin3-RING Ubiquitin Ligase Complexes. Darren Yong.

SU125
In-situ measurement of atomic displacement in TiO2 during flash sintering experiments. Bola Yoon.

SU126
Crystal structure of methylenetetrahydrofolate reductase (MTHFR) from Sphingobium sp. SYK-6. Hongyang Yu.

SU127
The crystal structure of RTFDC1 reveals a RING-like pseudoheterodimer responsible for pre-mRNA splicing regulation. Andrew Zhai.

SU128
Self-Assembled Three-Dimensional Deoxyribonucleic Acid (DNA) Crystals. Yue Zhao.

MO129
Molecular Replacement At SSGCID. Jan Abendroth.
MO130  
A micromanufactured dynamic beam-stop for continuous measurement of radiation dose. Marc Allaire.

MO132  
Recent developments and future of the GM/CA@APS X-ray crystallography user facility at the Advanced Photon Source. Michael Becker.

MO133  

MO134  
R&R – a de novo method to create search terms for IUCr documents. Tala-pady Bhat.

MO135  
Ligand binding mode determination in Fragment Based Drug Discovery using X-ray crystallographic data coupled with QM/MM based refinement: Further applications of XModeScore. Oleg Borbulevych.

MO136  
Ligand Validation for the Protein Data Bank. Stephen Burley.

MO137  

MO138  

MO139  
Molecular basis of CD22 Function and Therapeutic Targeting. June Ereno Orbea.

MO141  
Solving structures with native SAD on laboratory X-ray sources. Andreas Förster.

MO142  
The Canadian Light Source Annual Mx Data Collection School. James Gorin.

MO143  

MO144  
Shine Bright Like a Diamond: Microfocus X-ray Sealed Tube Sources with Diamond Hybrid Anode Technology. Juergen Graf.

MO145  

MO146  

MO147  
Tau overexpression substantially increase GFAT expression without direct interaction. Zhiqiang Hou.

MO148  
Microdiffraction Beamline NYX at NSLS-II. Seetharaman Jayaraman.

MO149  

MO150  
How new strategies can improve productivity in crystallization and cryoEM. Stefan Kolek.

MO152 CLS Mail-In Crystallography Highlights. Shaunivan Labiuk.


MO157 Tools and methods to ease the development of scripts for figure making in PyMOL. Blaine Mooers.


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