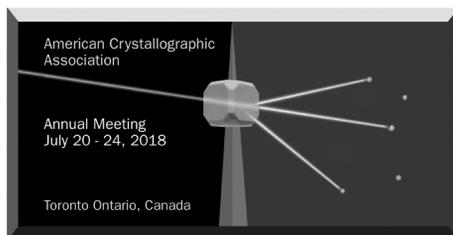


2018 ACA Annual Meeting



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

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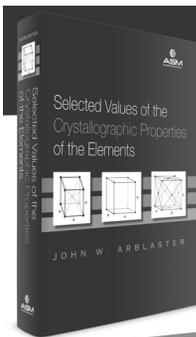
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CONTENTS

Sponsors.....	4
Exhibitors	6
Awards	9
General Information	10
Friday July 20	12
Saturday July 21	16
Sunday July 22.....	24
Monday July 23.....	30
Tuesday July 24.....	36
Wednesday July 25.....	42
Efter Student Lecturer Awards	43
Posters.....	44
Presenting Author Index	55



Selected Values of the Crystallographic Properties of the Elements

BY JOHN W. ARBLASTER | 684 PAGES | ISBN: 978-1-62708-154-2

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.

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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.]

Booth.....	Company
221.....	AIP Publishing/Structural Dynamics
219.....	American Institute of Physics
200.....	Amersterdam Scientific Instruments BV
111,113.....	Anatrace/Molecular Dimensions
202.....	Anton Paar Canada
306,308.....	Art Robbins Instruments
206.....	Avanti Polar Lipids Inc.
220.....	BioCAT
211,213,215.....	Bruker
303.....	Cambridge Crystallographic Data Centre
103.....	Canadian Light Source
319.....	CCP4 - STFC
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300.....	Douglas Instruments Ltd
203.....	Excillum AB
207,209.....	Formulatrix
301.....	Huber Diffraction USA
320.....	International Union of Crystallography
119.....	Lawrence Berkeley Laboratory - Advanced Light Source
214.....	Leica Microsystems
321.....	MacCHESS/Cornell University
314.....	Malvern Panalytical
311,313,315.....	MiTeGen, LLC
200.....	Nanome
201.....	NanoTemper Technologies
310.....	NatX-ray
115.....	Oxford Cryosystems Inc.
212.....	PROTO
218.....	RCSB PDB
107,109.....	Rigaku Americas
318.....	Southeast Regional Collaborative Access Team (SER-CAT)
302.....	STOE & Cie GmbH
309.....	Thermo Fisher Scientific
208.....	TTP LabTech Ltd.
307.....	Xenocs

**Exhibit Show
 Opening
 Friday, July 20th
 @ 7:30 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.

KEYNOTE



**Opening Ceremony with
plenary lecture by
1986 Nobel Laureate in Chemistry
John Polanyi**

**WHEN: Friday, July 20th @ 6:30 pm
WHERE: Grand Centre**

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>

GUEST SPEAKER

**The Annual Awards Banquet with special
guest speaker**

Natasha Myers

**WHEN: Tuesday, July 24th @ 6:30 pm
WHERE: Grand Centre**



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:

Friday July 20	7:30 AM - 7:30 PM
Saturday July 21	7:30 AM - 5:00 PM
Sunday July 22	7:30 AM - 5:00 PM
Monday July 23	7:30 AM - 5:00 PM
Tuesday July 24	7:30 AM - 12:00 PM

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:

Friday, July 20th
7:30 p.m. to 10:30 p.m.
[Show Closed from 12:00 p.m. to 2:00 p.m.]

Saturday, July 21st
10:00 a.m. to 7:30 p.m.
[Show Closed from 12:00 p.m. to 2:00 p.m.]

Sunday, July 22nd
10:00 a.m. to 7:30 p.m.
[Show Closed from 12:00 p.m. to 2:00 p.m.]

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]

FRIDAY | JULY 20

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 modeling 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

8:30 AM	Start
10:45-11:15 AM	Coffee Break
12:30-1:30 PM	Lunch
3:15-3:45 PM	Coffee Break
6:00 PM	End

FRIDAY | JULY 20

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.

SCHEDULE

8:30 AM	Start
10:30-10:45 AM	Coffee Break
11:30-12:30 PM	Lunch (On Your Own)
3:00-3:30 PM	Coffee Break
6:00 PM	End

FRIDAY | JULY 20

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 Merten & 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 rely 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

8:00 AM	Start
10:00-10:15 AM	Coffee Break
12:00-1:00 PM	Lunch
3:15-3:30 PM	Coffee Break
5:30 PM	End

FRIDAY | JULY 20

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

8:30 AM	Start
9:40 - 9:50 AM	Coffee Break
11:30 - 1:00 PM	Lunch
2:15-2:30 PM	Coffee Break
6:00 PM	End

FRIDAY EVENING ACTIVITIES

- 5:30 PM** **First Time Attendees
& Student Meeting Orientation
[Provincial North]**
- 6:30 PM** **Opening Reception
& Keynote Speaker
[Grand Centre]**
- 7:30 PM** **Exhibit Show Opening
[Osgoode & SHall A-F]**

SATURDAY | JULY 21

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 Soeipto.

Scheduled Time: 08:06
Arylsulfonyl Derivatives of 11-Azaarte-
misinin: Approaching New Polymorphs
via Seeds of Molecular Analogues.
Madiha Nisar.

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 it's 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 anti-
body responses against malaria trans-
mission-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

The use of Optical Microscopy and X-ray Powder and Single Crystal Diffraction to Identify and Structurally Characterize Novel Transition Metal Benzoates. Motunrayo Ladele.

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

X-Ray mapping in heterocyclic design. X-Ray diffraction study of the derivatives 5-amide-4,6-dimethylpyridone-2. Anna Kononenko.

Scheduled Time: 08:09

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

Scheduled Time: 08:12

Structural and functional characterization of bifunctional enzyme encoded by ribBX gene in riboflavin biosynthesis pathway of *Helicobacter pylori* 26695. Ruchi Gautam.

Scheduled Time: 08:15

Structure and Function of Terfestatin 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.

SATURDAY | JULY 21

Scheduled Time: 08:27

Structural determinants of varying innate immune pathway targeting in YopJ bacterial effectors. Jonathan Labriola.

Scheduled Time: 08:30

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

Scheduled Time: 08:33

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

Scheduled Time: 08:36

Surveillance of the nucleotide pool: Insights into the catalytic mechanism of mycobacterial antimutator protein MutT2. Amandeep Singh.

Scheduled Time: 08:39

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

T1: Transactions 1 - Shining a Light on Structure-Based Drug Design

Chairs: Steve Sossion & Vincent Stoll
Room: Grand Centre

Scheduled Time: 9:30 AM

Duration: 30 Minutes

IMCA-CAT: Accelerating Drug Discovery Through Synchrotron-Based Structural Biology

Lisa J. Keefe

IMCA-CAT / HWI

Scheduled Time: 10:00 AM

Duration: 30 Minutes

Systematic analysis of atomic protein-ligand interactions in the PDB

Mathieu Schapira

Structural Genomics Consortium

Scheduled Time: 11:00 AM

Duration: 30 Minutes

X-ray Free Electron Laser: Opportunities for drug discovery

Michael Hennig

LeadXpro AG

Scheduled Time: 11:30 AM

Duration: 30 Minutes

Achieving higher performance in high-throughput compound and fragment screening campaigns by the use of "Club Class" data collection with Pipedream and CRIMS

Gerard Bricogne

Global Phasing Limited

Scheduled Time: 12:00 PM

Duration: 30 Minutes

Using small molecule crystal structure data to improve drug discovery

Jason Cole

Cambridge Crystallographic Data Centre

T2: Transactions 2 - Shining a Light on Structure-Based Drug Design

Chairs: Steve Sossion & Vincent Stoll
Room: Grand Centre

Scheduled Time: 1:30 PM

Duration: 30 Minutes

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 Wedekind

University of Rochester School of Medicine & Dentistry

Scheduled Time: 2:00 PM

Duration: 30 Minutes

Fragment screening for a protein-protein interaction inhibitor to WDR5

Thomas Peat, CSIRO

Scheduled Time: 2:30 PM

Duration: 30 Minutes

Make the right measurement – discovery of an allosteric inhibition site for p300-HAT

Anna Gardberg

Constellation Pharmaceuticals

SATURDAY | JULY 21

Scheduled Time: 3:30 PM

Duration: 30 Minutes

Functional optimization of agonistic antibodies to OX40 receptor with novel Fc mutations to promote antibody multimerization

Mark J. Chiu

anssen Research & Development

Scheduled Time: 4:00 PM

Duration: 30 Minutes

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

Gil Privé

Princess Margaret Cancer Centre

Scheduled Time: 4:30 PM

Duration: 30 Minutes

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

Scheduled Time: 9:00 AM

Duration: 20 Minutes

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

Scheduled Time: 9:20 AM

Duration: 20 Minutes

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

Scheduled Time: 9:40 AM

Duration: 20 Minutes

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

Scheduled Time: 10:30 AM

Duration: 10 Minutes

How many conformers do you need?. James Holton.

Scheduled Time: 10:40 AM

Duration: 20 Minutes

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

Scheduled Time: 11:00 AM

Duration: 20 Minutes

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

Scheduled Time: 11:20 AM

Duration: 20 Minutes

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

Scheduled Time: 11:40 AM

Duration: 20 Minutes

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

Scheduled Time: 9:03 AM

Duration: 20 Minutes

Deciphering Nonenzymatic RNA Polymerization through Crystallography. Wen Zhang.

Scheduled Time: 9:23 AM

Duration: 12 Minutes

Structural and biochemical analyses of PadR-mediated transcriptional regulation. Sun Cheol Park.

SATURDAY | JULY 21

Scheduled Time: 9:35 AM
Duration: 25 Minutes
Using X-ray free electron laser to capture intermediate states. Yun-Xing Wang & Jason Stagno.

Scheduled Time: 10:30 AM
Duration: 25 Minutes
Emerging views of U2AF at the 3' splice site: A disease-relevant step of gene expression. Clara Kielkopf & Chandani Warnasooriya.

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 & Subhasg 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
Crystal Engineering of Photoreactive and Photosolvent Crystals. Jagadese Vittal.

Scheduled Time: 9:30 AM
Duration: 15 Minutes
Amphidynamic Behavior in Covalent Organic Frameworks probed via Powder X-ray Diffraction and ^{13}C CP-MAS T1 relaxation experiments. Demetrius Vazquez-Molina.21

Scheduled Time: 9:45 AM
Duration: 15 Minutes
Reversible Single Crystal-to-Single Crystal Phase Transition with Low-Temperature Induced Twinning of Diphenhydramine Citrate Salt. Kunlin Wang & Chenguang Wang.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
Photochemistry in nanocontainers. Yael Diskin-Posner & Linda L.J. Shimon.

Scheduled Time: 10:50 AM
Duration: 30 Minutes
Functional zwitterionic metal-organic frameworks with multi stimulus-responsive properties. Mario Wriedt & Darpandeep Aulakh.

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.

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

SATURDAY | JULY 21

Scheduled Time: 9:00 AM
Duration: 30 Minutes
The Fourth Ferroic: Ferrotoroidicity and Spherical Neutron Polarimetry. Efrain Rodriguez, Stephanie Gnewuch.

Scheduled Time: 9:30 AM
Duration: 15 Minutes
A Comparison of the Magnetic Structures of Candidate Ferrotoroidic Olivine Materials. Stephanie Gnewuch, Efrain Rodriguez.

Scheduled Time: 9:45 AM
Duration: 15 Minutes
Long range versus short range spin correlations in $A_{0.8}La_{1.2}MnO_{4.1}$ ($A = Sr, Ba$). Mirela Dragomir.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
Perovskite and Perovskite Related Iridates. Hans-Conrad zur Loye.

Scheduled Time: 10:50 AM
Duration: 30 Minutes
Magnetic order and spin dynamics of $j_{eff} = 1/2$ Ir⁴⁺ moments on the fcc lattice in $La_2B_{1-x}IrO_6$ ($B = Mg, Zn$). Adam Aczel.

Scheduled Time: 11:20 AM
Duration: 20 Minutes
Magnetic Moment Fragmentation in Nd_2ScNbO_7 . Christopher Wiebe.

Scheduled Time: 11:40 AM
Duration: 20 Minutes
 Dy_2ScNbO_7 : 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
Molecular Engineering of Crystalline Nano-optomechanical Transducers. Jacqueline Cole.

Scheduled Time: 3:45 PM
Duration: 15 Minutes
Visualization of 3D Diffraction: MAX3D Update. Jim Britten & Weiguang Guan.

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

Scheduled Time: 4:25 PM
Duration: 10 Minutes
Advancing in situ Dynamic Single-crystal X-ray Diffraction. Gage Bateman & Jason Benedict.

Scheduled Time: 4:35 PM
Duration: 15 Minutes
The magnitude of quanta from variance and intensity measurements. Wilfred Fullagar & Andrew Kingston.

SATURDAY | JULY 21

1.2.2 Hybrid Techniques

Chairs: Bhushan Nagar & Srinivas Chakravart

Room: Provincial North

Scheduled Time: 1:35 PM

Duration: 25 Minutes

Solving the phase problem in solution scattering. Thomas Grant.

Scheduled Time: 2:00 PM

Duration: 20 Minutes

Time-resolved SAXS using continuous-flow microfluidic mixers. Osman Bilsel, Srinivas Chakravarthy.

Scheduled Time: 2:20 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: 2:40 PM

Duration: 20 Minutes

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

Scheduled Time: 3:30 PM

Duration: 25 Minutes

Characterization of Monoclonal Antibodies Using X-ray and Neutron Scattering. Joseph Curtis.

Scheduled Time: 3:55 PM

Duration: 25 Minutes

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

Scheduled Time: 4:20 PM

Duration: 20 Minutes

Structural insights into the interaction of the conserved mammalian proteins GPR-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

Scheduled Time: 1:30 PM

Duration: 30 Minutes

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

Scheduled Time: 2:00 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: 2:30 PM

Duration: 30 Minutes

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

Scheduled Time: 3:30 PM

Duration: 20 Minutes

Structural Investigations into the Catalytic Mechanism of Human Manganese Superoxide Dismutase using Neutron and X-ray Crystallography. Jahaun Azadmanesh & William Lutz.

Scheduled Time: 3:50 PM

Duration: 20 Minutes

Vitamin E, Bilayer Asymmetry and Siloxane Lipids: Neutrons and X-rays Probing Different Membrane Problems. Drew Marquardt & Michael H.L. Nguyen.

Scheduled Time: 4:10 PM

Duration: 25 Minutes

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

SATURDAY | JULY 21

Scheduled Time: 4:35 PM

Duration: 25 Minutes

Improved Bragg Peak Integration for Neutron Crystallography by 3D Profile Fitting. Brendan Sullivan.

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

Chairs: Jing Tao & Albina Borisovich

Room: Provincial South

Scheduled Time: 1:30 PM

Duration: 25 Minutes

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

Scheduled Time: 1:55 PM

Duration: 15 Minutes

Probing Properties and Structure of Complex Oxides Superlattices using Scanning Electron Nanodiffraction. Roberto dos Reis & Weibing Yang.

Scheduled Time: 2:10 PM

Duration: 25 Minutes

Dynamical Calculations of Electron Diffraction for Crystals with incommensurate modulation. Lijun Wu & Yimei Zhu.

Scheduled Time: 2:35 PM

Duration: 15 Minutes

Challenges of micro electron diffraction in protein crystals. Neela Yennawar & Hemant Yennawar.

Scheduled Time: 3:20 PM

Duration: 25 Minutes

Probing laser-induced demagnetization dynamics in nanomaterials using ultrafast electron diffraction. Jianming Cao.

Scheduled Time: 3:45 PM

Duration: 25 Minutes

MeV Ultrafast Electron Scattering at SLAC: Status and Opportunities. Renkai Li, Suji Park.

Scheduled Time: 4:10 PM

Duration: 25 Minutes

Ultrafast Electron Diffuse Scattering: Mapping Momentum Dependent Electron-Phonon Coupling and Nonequilibrium Phonon Dynamics in 2D Materials. Bradley Siwick & Mark Stern.

1.3.1 Career Development

Chairs: René Coulombe

Room: Provincial North

SATURDAY EVENING ACTIVITIES

5:30 PM - 7:30 PM

SA Poster Session

[Osgoode & SHall A-F]

SUNDAY | JULY 22

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

Crystallography at Caltech 1980-1986. Bernie Santarsiero.

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

Remembering Dick Marsh. Jenny Glusker.

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

Refining the interface between automation and crystallisation. Janet Newman & Bevan Marshall.

Scheduled Time: 9:40 AM

Duration: 20 Minutes

Taking care of business: new drivers for crystallographic structure- and fragment-based drug discovery. Debanu Das.

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

High Throughput Protein-Ligand Complex Structure Solution with Phenix. Nigel Moriarty & Paul Adams.

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.

SUNDAY | JULY 22

Scheduled Time: 11:30 AM
Duration: 15 Minutes
Advancements in automated drop setting and imaging for high throughput crystallization. Mayank Aggarwal.

Scheduled Time: 11:45 AM
Duration: 15 Minutes
Advances in automated data analysis and processing within autoPROC, combined with improved characterization, mitigation and visualisation of the anisotropy of diffraction limits using STARANISO. Clemens Vonrhein, Ian J. Tickle.

2.1.3 NMR Crystallography

Chairs: Manish Mehta & Tomislav Friscic
Room: Provincial South

Scheduled Time: 9:05 AM
Duration: 30 Minutes
NMR Crystallography. Information on Structure, Symmetry, and Dynamics from Solid-State Multinuclear Magnetic Resonance Spectroscopy. David Bryce.

Scheduled Time: 9:35 AM
Duration: 25 Minutes
The Role of NMR Crystallography in Structure Verification of Organic Solids. Paul Hodgkinson.

Scheduled Time: 10:30 AM
Duration: 20 Minutes
New Pathways in NMR Crystallography: Structural Refinement and Solid-State NMR of the Periodic Table. Robert Schurko.

Scheduled Time: 10:50 AM
Duration: 25 Minutes
Hydrogen motional disorder in crystalline iron group chloride dihydrates. Philip Grandinetti.

Scheduled Time: 11:15 AM
Duration: 25 Minutes
What solid-state NMR can do to characterize metal-organic frameworks?. Yining Huang.

Scheduled Time: 11:40 AM
Duration: 20 Minutes
From Solid-State NMR to Crystal Structures through Combinatorial Tiling Theory. Darren Brouwer.

2.1.4 Advances in Biological Cryo-Electron Microscopy 1

Chairs: Wah Chiu & Lori Passmore
Room: Grand Centre

Scheduled Time: 9:00 AM
Duration: 30 Minutes
Single-Particle Cryo-EM Studies of Lipopolysaccharide Transport. Maofu Liao.

Scheduled Time: 9:30 AM
Duration: 15 Minutes
Structure of the Insulin Receptor in Complex with Insulin using Single Particle CryoEM Analysis. Giovanna Scapin.

Scheduled Time: 9:45 AM
Duration: 15 Minutes
Core components of bacterial protein secretion systems revealed at high resolution by cryo-electron microscopy. Justin Deme.

Scheduled Time: 10:30 AM
Duration: 30 Minutes
How is electrical signal generated? Structural and mechanistic investigations of Nav channels. Nieng Yan.

Scheduled Time: 11:00 AM
Duration: 15 Minutes
eBIC: Applying over 10yrs of software automation and support of MX beamlines to CryoEM. Alun Ashton, M Basham.

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 Isorecticular Metal Organic Frameworks. Wesley Newsome, Fernando 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.

Scheduled Time: 10:50 AM
Duration: 15 Minutes
Metal-Organic Frameworks as Platforms for the Nanostructuring of Single Molecule Magnets: New Insights from HRTEM. Juby Varghese, Darpandeep Aulakh.

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

Scheduled Time: 11:40 AM
Duration: 20 Minutes
Neutron Diffraction Study of Gas Adsorption and Separation in Metal-Organic Frameworks. 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
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. Graciela Diaz de Delgado, María Cecilia Dávila.

SUNDAY | JULY 22

Scheduled Time: 3:50 PM

Duration: 20 Minutes

Out of the Marsh and into the Swamp:
Validation of Powder Structures. Jim
Kaduk.

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 Chairs: J. Orgel & P. Langan Room: Provincial South

Scheduled Time: 1:30 PM

Duration: 45 Minutes

Contemporary and ancient tissues give
modern insights into biomedical engi-
neering. 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 struc-
tural 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 Madhurapan-
tula, Joseph Orgel.

2.2.3 General Interest - 1

**Chairs: Carla Sleboznick & Soumya
Remesh**

Room: Grand East

Scheduled Time: 1:30 PM

Duration: 15 Minutes

Removing residual bond density in or-
ganic molecules using simplified virtual
atoms: a technical note. Alexander
Nazarenko.

Scheduled Time: 1:45 PM

Duration: 15 Minutes

Temperature Validation using the CSD
Python API. Dean Johnston, Amy Sar-
jeant.

Scheduled Time: 2:00 PM

Duration: 15 Minutes

Extending 3-Dimensional Printed Rep-
resentations of Crystal Data: Printing
Anisotropic Models and Assembling
Structures Larger Than Your Print Tray.
Matthew Brown, Ken Van Wieren.

Scheduled Time: 2:15 PM

Duration: 15 Minutes

Investigating conformational land-
scapes through alternative cryocrystal-
lographic 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-depen-
dent kinases based on their donor
selectivity determinants revealed by
crystal structures. Masahiro Fujihashi,
Ryuhei Nagata.

SUNDAY | JULY 22

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

Evaluation of models in the 2016 Cryo-EM Model Challenge. Andriy Kryshtafovych, Catherine Lawson.

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

Structures and Mechanisms of Transcription Initiation and Its Regulation. Xiaodong Zhang.

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: Provincial North

Scheduled Time: 1:30 PM

Duration: 24 Minutes

Effect of addition of Lanthanum on the Hydrogen Storage Properties of TiFe Alloy. Md Alam, Pratibha Sharma.

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.

SUNDAY | JULY 22

Scheduled Time: 4:42 AM
Duration: 18 Minutes
New Layered Structures of Copper(II) and Silver(I) Salts of 4-Sulfobenzoic Acid. Philip Squattrito, Kelly Lambright.

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?. Dannielle 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

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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.

MONDAY | JULY 23

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
Structural vaccinology for malaria: Host-pathogen interactions, broadly-neutralizing antibodies and immunogen design. Niraj Tolia, Edwin Chen.

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
Structural characterization of adamantane-resistant mutants of the influenza M2 proton channel. Jessica Thomaston, William DeGrado.

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

Scheduled Time: 11:45 AM
Duration: 15 Minutes
Structure and function of the SEDS:bPBP bacterial cell wall synthesis machinery. Megan Sjødt.

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. Dorothee 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
Periodic structures beyond sphere packings: net, knots, polyvatenanes and weavings. Michael O'Keeffe.

Scheduled Time: 10:30 AM
Duration: 30 Minutes
Crystal Structure Prediction: From Topology to Geometry. Greg McCole.

Scheduled Time: 11:00 AM
Duration: 20 Minutes
IDEAL - Invariom Derived Electron Analysis for APEX3. Michael Ruf.

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
Aperiodic tilings, old and new -- an overflight. Shelomo Ben-Abraham.

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
Synchrotron single-crystal diffraction for chemistry and materials: new developments. William Clegg.

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
MetalJet Source for Time Resolved X-ray Diffraction and Scattering. Anasuya Adibhatla, Emil Espes.

Scheduled Time: 10:55 AM
Duration: 20 Minutes
MxDC, MxLIVE, and AutoProcess: Integrated User-friendly software for Synchrotron MX Beamlines. Kiran Mundboth.

Scheduled Time: 11:15 AM
Duration: 20 Minutes
Time-resolved Serial Synchrotron Crystallography: an efficient interlacing system enables milliseconds to seconds time delays. Pedram Mehrabi, Eike C. Schulz.

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
Tunable Structural and Optoelectronic Properties of Methylammonium Lead Bromide Perovskite under Pressure. Weizhao Cai, Rong Zhang.

Scheduled Time: 9:30 AM
Duration: 10 Minutes
Integrated solutions for most efficient in house high-pressure single crystal experiments. Martin Adam, Przemyslaw Dera.

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

MONDAY | JULY 23

Scheduled Time: 10:30 AM
Duration: 20 Minutes
Real-Time Monitoring of Shock-Driven Phase Transitions with Synchrotron X-ray Diffraction. Patricia Kalita, Seth Root.

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 Tisintite Formation and Its Implications for Impact Studies. Melinda Rucks, Matthew Whitaker.

Scheduled Time: 11:50 AM
Duration: 10 Minutes
High-Pressure/Temperature Behavior of the Alkali/Calcium Carbonate Shortite ($\text{Na}_2\text{Ca}_2(\text{CO}_3)_3$): Implications for Carbon Sequestration in the Deep Earth. Cara Vennari, Christin Beavers.

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.

MONDAY | JULY 23

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
Microgravity protein crystal growth for x-ray and neutron crystallography: What works and what would not!. Joseph Ng, James K. Baird.

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
Crystal Growth in Microgravity for Neutron Diffraction Studies. Timothy Mueser.

Scheduled Time: 4:20 PM
Duration: 20 Minutes
Growth of Large, Perfect Crystals of Human MnSOD for Neutron Crystallography. Gloria Borgstahl.

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
Search-match tool for atomic pair distribution functions and Crystallography Open Database. Pavol Juhas, Line Pouchard.

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
Quantifying local environment and structural similarity through order parameter-based site fingerprints and their application to machine learning. Nils Edvin Richard Zimmermann, Anubhav Jain.

MONDAY | JULY 23

Scheduled Time: 4:15 PM
Duration: 15 Minutes
Theoretical prediction of 5,5'-bistetrazole-1,1'-diolate (TKX-50) crystal structure. Xuehai Ju.

Scheduled Time: 4:30 PM
Duration: 15 Minutes
Theoretical Study of the Electronic Structure and Stability of Titanium Dioxide Clusters (TiO₂)_n with n=18, 28, and 38. Tania Gabriela Díaz Rodríguez, Gabriela Stephania Anaya González.

Scheduled Time: 4:45 PM
Duration: 15 Minutes
Computational investigation of Poisson's ratio and its relationship to crystal structure. John Dagdelen, Joseph Montoya.

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
The Physical Presence of Vitamin E in Lipid Membranes. Mitchell DiPasquale, Michael H.L. Nguyen.

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

Scheduled Time: 2:45 PM
Duration: 15 Minutes
Revealing the Hidden Relationship Between Pore-Forming Proteins and Biomembranes. Michael Nguyen.

Scheduled Time: 3:30 PM
Duration: 40 Minutes
Nanoscopy Domains in Model and Bacterial Membranes. John Katsaras.

Scheduled Time: 4:10 PM
Duration: 15 Minutes
Characterization of Self Assembled Hybrid Siloxane-phosphocholine Bilayers. Brett Rickeard, Mark Frampton.

Scheduled Time: 4:25 PM
Duration: 15 Minutes
X-ray and Neutron Scattering for Health and Disease. Maikel Rheinstadter.

Scheduled Time: 4:40 PM
Duration: 20 Minutes
Neutron Spin Echo Detects Effects of the pH-Low Insertion Peptide on Membrane Thickness Fluctuations. Haden Scott, Rana Ashkar.

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

MONDAY | JULY 23

Scheduled Time: 2:20 PM
Duration: 20 Minutes
Structural Distortions in Th-rich Fluorapatite. Joseph Chappell, John Rakovan.

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
The Gandolfi Stage: A Novel Approach for the Analysis of Single Crystals and Small Volume Samples. Gregory Schmidt.

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.

Scheduled Time: 7:15 PM
Duration: 40 Minutes
The Alliance for Diversity in Science and Engineering: Empowering graduate students. Steven Lopez.

MONDAY EVENING ACTIVITIES

5:00 PM

**All Members
Business Meeting
[Grand Centre]**

5:30 PM - 7:30 PM

**MO Poster Session
[Osgoode & SHall A-F]**

TUESDAY | JULY 24

**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
Duration: 30 Minutes
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
Duration: 15 Minutes
Cholera Toxin: Molecular Mechanisms
and Drug Design. Ute Krengel.

Scheduled Time: 9:45 AM
Duration: 15 Minutes
Structural basis of glycan specificity in
human rotaviruses. Liya Hu.

Scheduled Time: 10:30 AM
Duration: 30 Minutes
Microbial biofilms: Molecular mecha-
nisms to potential therapeutics. Lynne
Howell.

Scheduled Time: 11:00 AM
Duration: 15 Minutes
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 Bac-
terial LPS Transport. Christopher Koth,
Hoangdung Ho.

Scheduled Time: 11:45 AM
Duration: 15 Minutes
Structure of a Lipid-bound Viral Mem-
brane Assembly Protein Reveals a Novel
Modality for Interacting with Lipid Bilay-
er. 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 Assem-
bly for Robust Microcrystal Synchrotron
Crystallography. Qun Liu.

Scheduled Time: 9:20 AM
Duration: 20 Minutes
Metalloprotein Oxidation States Spatial-
ly 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 Co-
hen.

Scheduled Time: 11:00 AM
Duration: 20 Minutes
A High-Throughput Serial Crystallog-
raphy Beamline at CHESS. Doletha
Szebenyi, Aaron Finke.

TUESDAY | JULY 24

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 RLP2 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
In vivo carrier-driven crystallization for novel structural determinations. Kyle McDade.

Scheduled Time: 11:45 AM
Duration: 15 Minutes
Structure of the human Fe-S cluster assembly sub-complex: implications in Friedreich's ataxia and primary metabolism. Seth Cory.

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.

TUESDAY | JULY 24

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
The Small-Angle Scattering and HPLC-SAXS modules of the US-SOMO software suite. Mattia Rocco, Javier Pérez.

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
Operando In-Situ Microstructure & Structure Studies of Transformations in Advanced Materials. Andrew Allen, Fan Zhang.

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 Jafra.

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 Burtch.

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
Structural Transformation Begets Multiple Functions in the Viral Life Cycle. Michael Norris.

Scheduled Time: 1:55 PM
Duration: 20 Minutes
Shape Shifting in Apoptosis-Inducing Factor Allostery and Interactions: Switching between Oxidative Phosphorylation and Cell Death. John Tainer & Chris Brosey.

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.

TUESDAY | JULY 24

Scheduled Time: 2:35 PM

Duration: 25 Minutes

Another piece of the jigsaw: a new signaling axis defined by shape-specific RNR- hexamers. Yimon Aye.

Scheduled Time: 3:30 PM

Duration: 20 Minutes

Investigating the dynamic and complex oligomeric states of aldehyde dehydrogenase 7A1. David Korasick & Jack Tanner.

Scheduled Time: 3:50 PM

Duration: 25 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

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

4.2.2 General Interest - 2

Chairs: Michael Takase & Laura Van Staaldunen

Room: Grand East

Scheduled Time: 1:30 PM

Duration: 15 Minutes

Antibody Fab Fragments and their Crystal Organization. Travis Gallagher & Ioannis 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

Texture Analysis of Polycrystalline Vaterite Spherulites. Bryan Chakoumakos & Brenda Pracheil.

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

A Proposal for a Substrate - Assisted Catalytic Mechanism for Serine Peptidases. Michael N. James & Jiang Yin.

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.

TUESDAY | JULY 24

Scheduled Time: 4:30 PM
Duration: 15 Minutes
Atomic Insights into the Genesis of Cellular Filaments by Globular Proteins. Michael Sawaya & Laura McPartland.

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
Illustrating Key Concepts: Introducing Small Molecule Crystallography to Chemistry Undergraduates. Shao-Liang Zheng.

Scheduled Time: 1:55 PM
Duration: 20 Minutes
Mechanochemical Reactions and X-ray Powder Diffraction as a Teaching Tool. Karl Hagen.

Scheduled Time: 2:15 PM
Duration: 20 Minutes
Critical Mass: Organic-Organometallic Collaboration at the largest PUI. John Bender & Shannon Biros.

Scheduled Time: 2:35 PM
Duration: 25 Minutes
Pursuit of a NSF-MRI Funded Small-Molecule Single-Crystal X-ray Diffractometer at a PUI. Kraig Wheeler.

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
Everything Solid-State in Three Weeks: CHEM296 in January Term 2018. William Ojala.

Scheduled Time: 4:10 PM
Duration: 20 Minutes
Engaging Undergraduates in Crystallographic Research: "Structure of the Yersinia pestis UDP-glucose-1-phosphate uridylyltransferase". George Lountos & Morgan Gibbs.

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
Applications of X-ray Powder Diffraction in Pharmaceutical Industry. Rajni Bhardwaj.

TUESDAY | JULY 24

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
Real-time monitoring of mechano-chemical formation of pharmaceutical cocrystals using synchrotron X-ray diffraction. Luzia S. Germann & Mihails Arhangeliskis.

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
DFT Study of the Effect of Pressure on Framework Materials Including ZIF-8 and Inorganic zeolites. Wenlin Chen & Nancy Ross.

Scheduled Time: 1:45 PM
Duration: 15 Minutes
Synthesis, Characterisation, and Mesomorphic Properties of Some Novel Dicyanoheteropentacenes. Lana Hiscock & Louise Dawe.

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
Porous Framework Materials for Gas Separation: Mechanistic Investigation by Combining Neutron Crystallography and Computational Modeling. Wei Zhou.

Scheduled Time: 3:45 PM
Duration: 15 Minutes
X-Ray Diffraction and Computational Studies of a Series of Aryl Amides: Comparisons Between Molecular Structure in the Crystal State and in Isolation. Wayne Pearson & Joseph Urban.

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
How Crystallography in Synergy with Spectroscopy and Computation Catalyzed a Career in Chemical Crystallography. Joel Bernstein.

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 <i>Bacillus subtilis</i> 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 nanoconfinement
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 Nanostructuring 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 Isorecticular 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 Shonite ($\text{Na}_2\text{Ca}_2(\text{CO}_3)_3$): 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

POSTERS

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

Structural Characterization of the Helicobacter pylori Peptidyl-Prolyl cis,trans-Isomerase HP0175 Reveals an Extension of Chaperone Helices Upon Target Interaction. Gerald Audette.

SA2

Smyd2 Vs Smyd3: Structure based analysis of small molecule binding selectivity. Nithya Baburajendran.

SA3

Use of polysterism analysis to probe the conformational landscape and residue networks within an α -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

Design and Synthesis of Zwitterionic Metal-Organic Frameworks. Jenna Brockett.

SA7

Bonds, Symmetry and Virtual Atoms. David Brown.

SA8

Solid state structural transformation of two-dimensional coordination polymers. Robert Burrow.

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 FlhD 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.

POSTERS

SA17

Using topology of molecular solvation to enhance biomolecular structural refinement. George Giambasu.

SA18

Water structure in the intracellular osmosensor WNK1. El Goldsmith.

SA19

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

SA20

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

SA21

Volume-ensemble search models for molecular replacement. Dmytro Guzenko.

SA22

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

SA23

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

SA24

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

SA25

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

SA26

From X-ray Crystallography to Cryo-Electron Microscopy; Computing Infrastructure in Structural Biology. Jason Key.

SA27

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

SA28

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

SA29

X-Ray mapping in heterocyclic design. X-Ray diffraction study of the derivatives 5-amide-4,6-dimethylpyridone-2. Anna Kononenko.

SA30

Structure-based characterization and optimization of Eph receptor-targeting peptides. Bernhard Lechtenberg.

SA31

Accessing protein conformations of green fluorescent protein NowGFP at cryogenic and room temperature using X-ray crystallography. Ji-Hye Lee.

SA33

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

SA34

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

SA35

Deciphering the role of the Bateman domain in IMPDHs. H el ene Munier-Lehmann.

SA36

Fast Analytical Evaluation of Intermolecular Electrostatic Interaction Energies Using the Pseudoatom Representation of the Electron Density. Daniel Nguyen.

POSTERS

SA37

Arylsulfonyl Derivatives of 11-Azaarte-misinin: Approaching New Polymorphs via Seeds of Molecular Analogues. Madiha Nisar.

SA38

Everything Solid-State in Three Weeks: CHEM296 in January Term 2018. William Ojala.

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

Sulfur Dioxide-Halide Ion Complexes: A Crystallographic Investigation of Bonding. Katherine Robertson.

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

Crystalline Products of CO₂ Capture by Amines. Victoria Sena.

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 Soepto.

SA52

Experimental Electron Density Distribution of Tamoxifen Citrate. Edwin Stevens.

SA53

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

SA55

Probing the Structure of Axial Water Bound to Copper: An ESEEM Analysis of 17O-Water in Tutton Salt. Jacqueline Vitali.

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.

POSTERS

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

Effects of hydration and temperature on side-chain conformational heterogeneity in protein crystals. Hakan Atakisi.

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 Bragganolo.

SU65

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

SU66

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

SU67

Structural Analysis of Multiple Lab-Evolved Proteins that Bind HIV-1 TAR RNA with NanoMolar Affinity. Sai Shank 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 Terfestatin 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.

POSTERS

SU75

Crystallization of Novel Polyglycine Hydrolases from two fungal families: *Epicoccum sorghi* and *Fusarium solani*. Nicole Fraser.

SU76

Structural and functional characterization of bifunctional enzyme encoded by *ribBX* gene in riboflavin biosynthesis pathway of *Helicobacter pylori* 26695. Ruchi Gautam.

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 μ 2-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

Structural determinants of varying innate immune pathway targeting in YopJ bacterial effectors. Jonathan Labriola.

SU91

The use of Optical Microscopy and X-ray Powder and Single Crystal Diffraction to Identify and Structurally Characterize Novel Transition Metal Benzoates. Motunrayo Ladele.

SU92

Substrate specificity of N-methyltransferases in benzylisoquinoline alkaloid metabolism. Dean Lang.

POSTERS

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. pectinatus* by X-ray Crystallography. Darya Marchany-Rivera.

SU98

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

SU99

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

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.

SU102

Crystal Structure and Cytotoxic Assay of a Novel Potential Anticancer Chalcone. Hamilton Napolitano.

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.

SU105

Structural Determination of ATP citrate lyase. Vinh Nguyen.

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.

SU108

Assessment of Structural Features in Cryo-EM Density Maps using SSE and Side Chain Z-Scores. Greg Pintilie.

SU109

Overexpression, purification of GSK3 and its 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.

POSTERS

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

Surveillance of the nucleotide pool: Insights into the catalytic mechanism of mycobacterial antimutator protein MutT2. Amandeep Singh.

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 AIPL1 and its TPR domain in Leber congenital amaurosis 4 (LCA4) a severe form of childhood blindness. Ravi Prakash Yadav.

SU122

Characterization of C-terminal structure of MinC and its implication in evolution of bacterial cell division. Shaoyuan Yang.

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.

POSTERS

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

Performance without the Pain, Extending the Capabilities of Low-Maintenance Home-Lab Systems for Biological Crystallography. Matthew Benning.

MO134

R&R -a de novo method to create search terms for IUCr documents. Talapady 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

Evaluation of New PHOTON III Detectors for Chemical Crystallography Applications. Charles Campana.

MO138

Using Scipion for Stream Image Processing at CryoEM Facilities. Jose Miguel de la Rosa Trevin.

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

The MORPHEUS III protein crystallization screen: at the frontier of drug discovery. Fabrice Gorrec.

MO144

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

MO145

IUCr – Supporting Crystallography Around the World. Marvin Hackert.

MO146

BioXTAS RAW: a free open-source program for small-angle X-ray scattering data reduction and analysis. Jesse Hopkins.

MO147

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

MO148

Microdiffraction Beamline NYX at NSLS-II. Seetharaman Jayaraman.

MO149

A Comparison of Gas Stream and Plunge Cooling in Macromolecular Cryocrystallography. Douglas Juers.

MO150

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

POSTERS

MO151

Northeastern Collaborative Access Team (NE-CAT) Crystallography Beam Lines for Challenging Structural Biology Research. Igor Kourinov.

MO152

CLS Mail-In Crystallography Highlights. Shaunivan Labiuk.

MO153

The Rigaku Oxford Diffraction XtaLAB Synergy-S, a versatile microfocussed tube diffractometer for weakly diffracting samples. Pierre Le Magueres.

MO154

A Low Cost Low-temperature Crystal Mounting Device. Vincent Lynch.

MO156

Structural insights on three series of anti-malarial N-myristoyltransferase inhibitors. Stephen Mayclin.

MO157

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

MO158

IMCA-CAT Advanced Photon Source Facility for Structure-Based Drug Discovery. Anne Mulichak.

MO159

CMCF-ID: A versatile high-flux and micro-focusing beamline for macromolecular crystallography. Kiran Mundboth.

MO160

Molecular basis for PNAG-dependent biofilm disruption by PgaB. Roland Pfoh.

MO161

Assessment of Structural Features in Cryo-EM Density Maps using SSE and Side Chain Z-Scores (Updated). Grigore Pintilie.

MO162

Structure-based discovery and optimization of inhibitors for the class D-lactamase OXA-24/40. Rachel Powers.

MO163

An update on detergent usage in Cryo-EM structure determination of membrane proteins. Edward Pryor.

MO164

Dose-sliced data collection; Get the best from that crystal!. Kanagalaghatta Rajashankar.

MO165

Recent Developments at the Beamline for Biological Small Angle X-ray Scattering BL4-2 at SSRL. Ivan Rajkovic.

MO167

Using Modelling and Docking to Search for the Natural Ligand of COUPTFI. Ross Reynolds.

MO168

Announcing the ACA Best Practices for Data Analysis & Archiving Scientific Interest Group. John Rose.

MO169

The Collaborative Crystallography program at the Advanced Light Source. Banumathi Sankaran.

MO170

Structural Basis of Interaction of Herpesvirus Proteins with the Deubiquitinase USP7. Vivian Saridakis.

MO171

Iffy imidazoles: misplaced hydrogen atoms and undetected disorder. Carl Schwalbe.

MO172

Crystallization strategy when no well-diffracted crystals are obtained in the crystallization screening. Miki Senda.

MO173

Structure-based integrated approach for analysis of the GTP metabolism. Toshiya Senda.

MO174

Industrial Macromolecular and Small Molecule Crystallography at the Canadian Light Source. Denis Spasyuk.

MO175

Synthetic glycopeptide selected by directed evolution in complex with anti-HIV-1 Fab 2G12. Robyn Stanfield.

MO177

Impact of Disease-Linked Mutations on the Structure and Activity of Aldehyde Dehydrogenase 7A1 (ALDH7A1). John Tanner.

MO178

Unveiling a Drift Resistant Cryptotope within Marburgvirus Nucleoprotein Recognized by Llama Single-domain Antibodies. Alex Taylor.

MO181

New Developments of X-ray diffraction and pair distribution function beamlines 11-ID and 17-BM at Advanced Photon Source. Wenqian Xu.

MO182

RCSB Protein Data Bank: Sustaining a Living Digital Data Resource that Enables Breakthroughs in Scientific Research and Biomedical Education. Christine Zardecki.

MO183

DECOR: The Database of Educational Crystallographic Online Resources. Michael Zdilla.

PRESENTING AUTHOR INDEX

- Abbas, Yazan..... PS2
 Abendroth, Jan PS3
 Abraham, Shelomo..... 3.1.3
 Aczel, Adam..... 1.1.4
 Adam, Martin..... 3.1.5
 Adibhatla, Anasuya..... 3.1.4
 Afonine, Pavel 1.1.1
 Aggarwal, Mayank 2.1.2
 Alam, Md..... 2.2.5
 Allaire, Marc..... PS3
 Allen, Andrew 4.1.5
 Arturo, Emilia 3.2.1
 Ashton, Alun..... 2.1.4
 Atakisi, Hakan PS2
 Audette, Gerald..... PS1
 Aye, Yimon 4.2.1
 Azadmanesh, Jahaun 1.2.3
 Baburajendran, Nithya PS1
 Bamford, Natalie PS2
 Bateman, Gage..... 1.2.1
 Bateman, Tom PS2
 Beamer, Lesa PS1
 Beavers, Christine 2.3.1, PS1
 Becker, Stefan..... PS1
 Becker, Michael..... PS3
 Bedem, Henry 1.1.1
 Bender, John 4.2.3
 Benning, Matthew..... PS3
 Bernstein, Herbert..... 4.1.2
 Bernstein, Joel..... 4.2.5
 Bhardwaj, Rajni..... 4.2.4
 Bhat, Talapady PS3
 Billinge, Simon 3.2.3, PL1
 Bilsel, Osman 1.2.2
 Bogdanov, Georgii 2.2.5
 Borbulevych, Oleg PS3
 Borgstahl, Gloria 3.2.2
 Bowman, Sarah 2.2.3
 Bragagnolo, Nicholas PS2
 Bricogne, Gerard T1
 Bridges, Craig 4.1.5
 Britten, Jim 1.2.1
 Brock, Carolyn 2.2.1
 Brockett, Jenna PS1
 Brouwer, Daren 2.1.3
 Brown, Matthew 2.2.3
 Brown, David PS1
 Bryce, David 2.1.3
 Bu, Zimei 1.2.3, 4.1.4
 Buchanan, Susan 3.1.1
 Bulut, Haydar PS2
 Burley, Stephen..... 3.1.2
 Burrow, Robert PS1
 Burtch, Nicholas..... 4.1.5
 Byram, Susan..... 2.1.1
 Cai, Weizhao 3.1.5
 Campana, Charles PS3
 Campbell, Branton PS1
 Cao, Jianming 1.2.4
 Carbone, vince PS1
 Carta, Veronica..... PS1
 Case, David 1.1.1
 Castañeda, Raúl..... 4.1.3
 Chagas, Marcio PS2
 Chakoumakos, Bryan 4.2.2
 Chakraborty, Indranil..... PS1
 Chappell, Joseph..... 3.2.5
 Chavali, Sai PS2
 Chen, Lin 1.2.1
 Chen, Wenlin 4.2.5
 Chergui, Majed 1.2.1
 Childers, Kenneth PS2
 Chiu, Mark..... T2
 Cho, So PS1
 Chu, Sam..... PS2
 Chung, Ivy..... PS2
 Ciston, Jim 1.2.4
 Clegg, William 3.1.4
 Cleveland, Thomas 1.2.3
 Clinger, Jonathan..... PS2
 Cohen, Aina 4.1.2
 Colbert, Christopher 1.2.2
 Cole, Jacqueline..... 1.2.1
 Cole, Jason T1
 Cordeiro, Raquel..... PS2
 Corfield, Peter..... 4.1.3
 Cory, Seth..... 4.1.3
 Criswell, Angela..... 1.2.2
 Curtis, Joseph 1.2.2
 Custodio, Jean PS2
 Cuypers, Maxime PS2
 Dagdelen, John 3.2.3
 Das, Debanu..... 2.1.2
 Davarinejad, Hossein PS1
 Dawe, Louise 2.3.1
 Dawe, Louise 4.2.3
 Day, Maxwell 3.2.5
 Degen, Thomas 4.1.5

PRESENTING AUTHOR INDEX

- Delgado, Graciela 2.2.1
 Deme, Justin 2.1.4
 DeWhitt, Kristofer 3.2.2
 DiPasquale, Mitchell 3.2.4
 Dragomir, Mirela 1.1.4
 Eckert, Juergen 4.2.5
 Emsley, Paul 3.1.2
 Falvello, Larry 2.2.1
 Fan, Lixin PS1
 Ferrer, Jean 2.1.2
 Fischmann, Thierry 3.1.2
 Fitzgibbons, Thomas 4.1.5
 Fodje, Michel PS3
 Fortes, Dominic 2.2.5
 Foxman, Bruce 4.2.5
 Fraser, Nicole PS2
 Friscic, Tomislav 1.2.1, 2.1.5
 Fronczek, Frank 2.2.1
 Fujihashi, Masahiro 2.2.3
 Fullagar, Wilfred 1.2.1
 Gagné, Olivier 3.2.5
 Gallagher, Travis 4.2.2
 Gardberg, Anna T2
 Garman, Elspeth 4.1.2
 Gassensmith, Jeremiah 2.1.5
 Gautam, Ruchi PS2
 Gerasimchuk, Nick 4.2.2
 Germann, Luzia 4.2.4
 Gerstein, Mark 3.2.1
 Ghassemi, Omid PS1
 Gheorghita, Andreea PS2
 Giambasu, George PS1
 Gildenberg, Melissa PS2
 Gilman, Morgan PS2
 Gindhart, Amy 4.2.4
 Ginell, Garrett PS2
 Ginn, Helen 1.1.1
 Giulianotti, Marc 3.2.2
 Glusker, Jenny 2.1.1
 Gnewuch, Stephanie 1.1.4
 Goldsmith, Elizabeth PS1
 Golen, James PS1
 Golzarroshan, Bagher PS2
 Gorin, James PS3
 Gorrec, Fabrice PS3
 Graf, Juergen PS3
 Grandinetti, Philip 2.1.3
 Grant, Thomas 1.2.2
 Gray, Danielle 2.3.1
 Guillot, Michael PS1
 Guo, Shuaiqi 4.1.3
 Gupta, Kushol 4.2.1
 Guzei, Ilia 3.2.2
 Guzenko, Dmytro PS1
 Hackert, Marvin PS3
 Hagen, Karl 4.2.3
 Halgas, Ondrej PS2
 Haller, Joseph PS2
 Haller, Jeffrey PS2
 Harada, Ayaka PS1
 Hart, Gus 3.2.3
 Hawthorne, Frank PL2
 Heberle, Frederick 3.2.4
 Hennig, Michael T1
 Hillard, Elizabeth 4.2.5
 Hiscock, Lana 4.2.5
 Hodgkinson, Paul 2.1.3
 Hofer, Pascal PS3
 Holton, James 1.1.1
 Hopkins, Jesse PS3
 Hou, Zhiqiang PS3
 Howell, Lynne 4.1.1
 Hruza, Alan PS1
 Hu, Liya 4.1.1
 Hu, Chunhua 4.2.5
 Huang, Yining 2.1.3
 Huang, Ji PS2
 Hützler, Wilhelm PS1
 Irving, Thomas 2.2.2
 Jaffe, Eileen 3.2.1
 James, Michael 4.2.2
 Jayaraman, Seetharaman PS3
 JHA, Vikash PS2
 Jin, Tengchuan 4.2.2
 Johnson, Rachel PS2
 Johnston, Dean 2.2.3
 Ju, Xuehai 3.2.3
 Juers, Douglas PS3
 Juhas, Pavol 3.2.3
 Jung, Dubravka 2.2.5
 Kabova, Elena 4.2.4
 Kaduk, Jim 2.2.1, 4.2.4
 Kaduk, James PS1
 Kalita, Patricia 3.1.5
 Katsaras, John 3.2.4
 Kay, Julie 3.2.1
 Ke, Ailong 1.1.2
 Keefe, Lisa T1

PRESENTING AUTHOR INDEX

- Key, Jason PS1
 Khalifah, Peter 3.1.3
 Kielkopf, Clara 1.1.2
 Kim, Jin PS1
 Kim, meong PS2
 Kinnibrugh, Tiffany PS1
 Kirby, Nigel 4.1.4
 Kolek, Stefan PS3
 Kononenko, Anna PS1
 Korasick, David 4.2.1
 Koth, Christopher 4.1.1
 Kourinov, Igor PS3
 Kregel, Ute 4.1.1
 Kryshchak, Andriy 2.2.4
 Kung, Yan 4.2.2
 KWON, DO PS2
 Labiuk, Shaunivan PS3
 Labriola, Jonathan PS2
 Ladele, Motunrayo PS2
 Lander, Gabriel 2.2.4
 Lang, Dean PS2
 Langan, Paul 2.2.2
 Lany, Stephan 3.2.3
 Lawson, Catherine 2.2.3
 Lechtenberg, Bernhard PS1
 Lee, Ji PS1
 Lee, Choongdeok PS2
 Lehmann, H el ene PS1
 Li, Renkai 1.2.4
 Li, Yan PS1
 Li, Zhijie PS1
 Liao, Maofu 2.1.4
 Liebschner, Dorothee 3.1.2
 Lin, Chang PS2
 Liu, Qun 4.1.2
 Logan, Matthew 2.1.5
 Logan, Baker PS1
 Lopez, Steven 3.3.1
 Lountos, George 4.2.3
 Lovelace, Jeffrey 2.2.3
 Loye, Hans 1.1.4
 Lynch, Vincent PS3
 Madhurapantula, Rama 2.2.2
 Magueres, Pierre PS3
 Maji, Debanjana PS2
 Marquardt, Drew 1.2.3
 Mayclin, Stephen PS3
 McAuliffe, Rebecca 4.1.5
 McCallum, Matthew PS2
 McColm, Greg 3.1.3
 McDade, Kyle 4.1.3
 McLaughlin, Krystle 4.2.3
 McLellan, Jason PL3
 McLeod, Matt 2.2.3
 McLeod, Brandon PS2
 Mehrabi, Pedram 3.1.4
 Meisburger, Steve 1.1.1
 Mesbah, Adel 3.2.5
 Messerschmidt, Marc 1.2.1
 Mitchell, Travis 1.1.3, PS1
 Moiani, Davide PS2
 Molina, Demetrius 1.1.3
 Montemayor, Eric 1.1.2
 Mooers, Blaine 4.1.4, PS3
 Moreau, David 2.2.3
 Moriarty, Nigel 2.1.2
 Mueser, Timothy 1.2.3
 Mueser, Timothy 3.2.2
 Mulichak, Anne PS3
 Mundboth, Kiran 3.1.4
 Murphy, Michael 4.1.1
 Murshudov, Garib 1.1.1
 Nagal, Kiyoshi 2.2.4
 Nagao, Michihiro 3.2.4
 Nambisan, Anand PS2
 Napolitano, Hamilton PS2
 Nava, Nardo PS2
 Nazarenko, Alexander 2.2.3
 Newman, Janet 2.1.2
 Newsome, Wesley 2.1.5
 Newton, Jocelyn PS2
 Ng, Joseph 3.2.2
 Ng, Kenneth 4.1.3
 Nguyen, Michael 3.2.4
 Nguyen, Daniel PS1
 Nguyen, Vinh PS2
 Nisar, Madiha PS1
 Noble, Schroeder PS2
 Noll, Bruce 4.2.2
 Norris, Michael 4.2.1
 Nurizzo, Didier 2.1.2
 O'Keeffe, Michael 3.1.3
 Ojala, William 4.2.3, PS1
 Orbea, June PS3
 Orgel, Joseph 2.2.2
 Packianathan, Charles PS2
 Pagola, Silvina 4.2.4
 Palzkill, Timothy 4.1.1
 Park, Sun 1.1.2
 Partch, Carrie PS1

PRESENTING AUTHOR INDEX

- Pearson, Wayne 4.2.5
 Peat, Thomas T2
 Peng, Shuxia 4.1.1
 Pernot, Petra 3.1.4
 Petersen, Emma 3.1.5
 Pfoh, Roland PS3
 Pintilie, Greg PS2
 Pintilie, Grigore PS3
 Posner, Yael 1.1.3
 Powers, Rachel PS3
 Prescher, Clemens 3.1.5
 Privé, Gil T2
 Pryor, Edward PS3
 Pujari, Narsimha PS2
 Rae, Alan 3.2.5
 Rahighi, Simin PS1
 Rajashankar, Kanagalaghatta PS3
 Rajkovic, Ivan PS3
 Raman, Swetha PS1
 Rawn, Claudia PS1
 Read, Randy 1.1.1
 Reichert, Paul 3.2.2
 Reid, Joel 4.2.4
 Reis, Roberto 1.2.4
 Remesh, Soumya 1.1.2
 Reynolds, Ross PS3
 Rheinstadter, Maikel 3.2.4
 Richardson, Jane 2.2.4
 Riccard, Brett 3.2.4
 Rigin, Sergei 2.2.5
 Ringe, Dagmar 1.2.3
 Rivera, Darya PS2
 Robertson, Katherine PS1
 Rocco, Mattia 4.1.4
 Rodriguez, Efrain 1.1.4
 Rodriguez, Tania 3.2.3
 Romo, Fernando 2.1.5
 Rose, John PS3
 Ross, Nancy 3.2.5
 Rucks, Melinda 3.1.5
 Ruetf, Uta 2.1.5
 Ruf, Michael 3.1.3
 Rutherford, Megan 1.1.4
 Sagar, Vatsala PS2
 Sankaran, Banumathi PS3
 Santarsiero, Bernie 2.1.1
 Saper, Mark 4.2.1
 Saridakis, Vivian PS3
 Sarmiento, Janeth 2.2.5
 Sauter, Nicholas 4.1.2
 Sawaya, Michael 4.2.2
 Scally, Stephen 3.1.1
 Scapin, Giovanna 2.1.4
 Scapin, Giovanna T2
 Schapira, Matthieu T1
 Schmidt, Gregory 3.2.5
 Schnicker, Nicholas 4.2.2
 Schuller, David PS1
 Schuman, Brock PS2
 Schurko, Robert 2.1.3
 Schwalbe, Carl PS3
 Scott, Haden 3.2.4
 Sears, Jeffrey PS1
 Seiler, Vanessa PS1
 Sena, Victoria PS1
 Senda, Miki PS3
 Senda, Toshiya PS3
 Shamsi, Tooba PS2
 Shek, Roger PS2
 Sheldrick, George 2.2.1
 Shivakumaraswamy, Santosh PS2
 Simmons, Chad PS1
 Sims, Melissa 3.1.5
 Singh, Amandeep PS2
 Siwick, Bradley 1.2.4
 Sjødt, Megan 3.1.1
 Skrynnikov, Nikolai 4.2.2
 Sleboznick, Carla 3.1.5
 Smith, Stacey 4.1.3
 Soares, Alexei 2.1.2
 Soecripto, Aristyo PS1
 Soldatov, Dmitriy 2.2.3
 song, wanseok PS2
 Sosnick, Tobin 1.2.2
 Spasyuk, Denis PS3
 Spek, Anthony 2.1.1
 Squatrito, Philip 2.2.5
 Stan, Camelia 3.2.5
 Stanfield, Robyn PS3
 Stephens, Peter 4.2.4
 Stevens, Edwin PS1
 Stiers, Kyle 3.2.1
 Strutz, Wyatt PS3
 Strynadka, Natalie 2.1.4
 Sullivan, Brendan 1.2.3
 Sutter, Markus 4.2.2
 Sverzhinsky, Aleksandr PS2
 Szebenyi, Doletha 4.1.2
 Tainer, John 4.2.1
 Takagi, Yuichiro PS1

PRESENTING AUTHOR INDEX

- Tanaka, Hiroaki 3.2.2
 Tanner, John 3.1.2
 Tanner, John PS3
 Tanski, Joe 2.3.1
 Taylor, Alex PS3
 Terwilliger, Thomas PS3
 Thomas, William 4.2.1
 Thomaston, Jessica 3.1.1
 Thorn, Andrea PS3
 Timofeeva, Tatiana 4.1.3
 Tolia, Niraj 3.1.1
 Tomás, Milagros 4.2.5
 Toney, Michael 4.1.5
 Topi, Filip 1.1.3
 Torres, Miguel PS2
 Trevin, Jose PS3
 Udovic, Boris 2.2.5
 Urban, Volker 2.2.2
 Uthoff, Matthias PS2
 Vance, Tyler PS2
 Vargas, Javier 2.2.4
 Varghese, Juby 2.1.5
 Vennari, Cara 3.1.5
 Vitali, Jacqueline PS1
 VITAL, Jagadese 1.1.3
 Vonrhein, Clemens 2.1.2
 Wang, Yun 1.1.2
 Wang, Kunlin 1.1.3
 Wang, Bi 2.1.1
 Wang, Xiaoping 4.1.5
 Ward, Suzanna 2.1.1
 Washington, Talitha 3.3.1
 Watkins, Maxwell 4.1.4
 Watson, Jeff 4.2.1
 Wedekind, Joseph PS1
 Wedekind, Joseph T2
 Westerhoff, Lance 2.2.3
 Wheeler, Craig 4.2.3
 Whitaker, Matthew 3.1.5
 Whitley, Matthew 3.2.1
 Wiebe, Christopher 1.1.4
 Wiess, Thomas 4.1.4
 Wilk, Piotr 3.2.1
 Wilson, Ian 3.1.1
 Woll, Kellie PS1
 Wriedt, Mario 1.1.3
 Wu, Lijun 1.2.4
 Wu, Hui 2.1.5
 Xu, Zhen 1.2.2
 Xu, Wenqian PS3
 Yadav, Ravi PS2
 Yamamoto Masaki 4.1.2
 Yan, Nieng 2.1.4
 Yang, Shaoyuan PS2
 Yang, Yidai PS2
 Ye, Qilu PS1
 Yennawar, Neela 1.2.4
 Yong, Darren PS2
 Yoon, Bola PS2
 Young, Victor 2.2.1, 2.3.1
 Yu, Hongyang PS2
 Yue, Wyatt 3.2.1
 Zardecki, Christine PS3
 Zavalij, Peter 4.2.2
 Zdilla, Michael PS3
 Zhai, Andrew PS2
 Zhang, Wen 1.1.2
 Zhang, Xiaodong 2.2.4
 ZHANG, Huawei PS1
 Zhao, Rui 2.2.4
 Zhao, Yue PS2
 Zheng, Shao 4.2.3
 Zhou, Wei 4.2.5
 Ziletti, Angelo 3.1.3
 Zimmermann, Nils 3.2.3
 Zuo, Jian PS1

NOTES