



# **ANNUAL MEETING**

**July 25-30, 2009  
Toronto, Canada**

# ***Program***

[www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)



# 2009 Annual Meeting July 25 - 30 Toronto, Ontario Canada Sheraton City Centre Hotel

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[www.AmerCrystalAssn.org](http://www.AmerCrystalAssn.org)

## About the ACA

The American Crystallographic Association (ACA) was founded in 1949 through a merger of the American Society for X-Ray and Electron Diffraction (ASXRED) and the Crystallographic Society of America (CSA). The objective of the ACA is to promote interactions among scientists who study the structure of matter at atomic (or near atomic) resolution. These interactions will advance experimental and computational aspects of crystallography and diffraction. They will also promote the study of the arrangements of atoms and molecules in matter and the nature of the forces that both control and result from them.

Membership in the ACA is open to any person who is actively interested in the purposes of the Association and whose application is approved by the ACA Council or its designee. All members are entitled to voting privileges. Student members are very welcome and their contributions to the life and vigor of the association has always been important. The benefits of membership are the same in all categories. These include: voting privileges, RefleXions, the ACA newsletter that is published 4 times per year, complimentary subscription to the Newsletter of the International Union of Crystallography, and Physics Today, a monthly publication of AIP, and reduced rates for the International Tables for X-Ray Crystallography, Structure Reports, Journal of Applied Crystallography, and Acta Crystallographica when purchased for the member's personal use only. The ACA is a member society of the American Institute of Physics (AIP) and an Affiliate Member of the International Union of Crystallography.

The total membership of the ACA is about 2,200. National meetings are held annually. There are 12 Special Interest Groups (SIG's) concerned with Biological Macromolecules, Fiber Diffraction, General Interest, Industrial, Materials Science, Neutron Scattering, Powder Diffraction, Service Crystallography, Small Angle Scattering, Small Molecules, Synchrotron Radiation and Young Scientists. Members may join as many of these groups that are of interest them. Each Special Interest Group is responsible for organizing sessions at Annual Meetings at least every other year.

The headquarters of the association is located at Hauptman Woodward Medical Research Institute, 700 Ellicott St., Buffalo, NY 14203.

# FRIDAY & SATURDAY, JULY 24 & 25

## WK.01 JANA - Incommensurate Crystal Structures

Chairs: Jim Kaduk, Olivier Gourdon

Essex Ballroom

Jana2006[1] is the last generation of the computing system Jana. Its development has started in early eighties when Václav Petříček developed several programs for analysis of three-dimensional structures from single-crystal X-ray diffraction data known as the SDS system. Later on, during the stay in Buffalo, USA, he wrote program Jana specialized to refinement and Fourier calculations for modulated structures. Both systems were developing separately until 1998 when they have been merged into a universal system Jana98. Another important milestone was adding a support for powder refinement in 2001 and possibility of an arbitrary combination of data sources in 2006. Jana system has currently about 1300 registered users around the world and it is almost exclusive tool for solution of modulated and composite structures.

In the field of basic crystallography Jana2006 offers usual tasks like automatic determination of space group, searching for higher symmetry, calling of SIR or Superflip[2] for structure solution, evaluation of Fourier maps, adding of hydrogen atoms etc. Advanced tools can be used for transformations, calculation of gener-

ally oriented Fourier sections, definition of twinning or rigid bodies, multiphase refinement, multipole refinement, introduction of local symmetry etc. Jana2006 can combine multiple data such as powder and/or single crystal diffraction data from X-ray, synchrotron and neutron diffraction.

The main focus of this workshop is the use of Jana2006 to investigate the atomic arrangement in Incommensurate structures. Such structures can be investigated up to the dimension 3+3. The superspace symmetry can be found from the diffraction pattern using the same semi-automatic tools like for standard structures. Jana2006 offers traditional harmonic modulation functions for occupancy, position and ADP as well as discontinuous functions (crenel and sawtooth). In the crenel-like description the positions and ADP parameters can also be described with Legendre polynomials. The modulated structures can be visualized by calling an external plotting program for a structure transformed to P1 symmetry, by plotting modulated parameters as function of t coordinate or by investigating two-dimensional sections by 3+d-dimensional Fourier map. For solution of modulated structures Jana2006

can directly call program Superflip based on charge flipping which can also be used for verification of superspace symmetry. Commensurate structures represent very useful concept for description of structure families. Jana2006 can determine a supercell symmetry corresponding to the t value used for the calculation and it can transform commensurate structure for a given t to the equivalent three-dimensional supercell. Composite (or intergrown) structures are also supported. Finally, the latest version of Jana2006 contains a convertor between representation analysis and magnetic (super)space groups which enables crystallographic approach to magnetic structures. This two days workshop will be composed of 45mn lectures as well as practical exercises. The main goal is to give to all participants an expertise on modulated structures with the advanced tools than JANA2006 can offer. During the first half day, using single crystal and powder diffraction data of a simple structure we shall present the basic "philosophy" of the program. The rest of the workshop will deal with simple modulated structures and finally during the last more advanced cases.

### Schedule

#### 1st halfday

Lecture 1 - Michal Dušek, Václav Petříček  
Presentation of all the features of Jana2006  
Exercise 1 .Advanced 3d example

#### 2nd halfday

Lecture 2 - Václav Petříček  
Introduction to superspace  
Exercise 2 .Simple (3+1)d example

#### 3rd and 4th halfday

Lecture 3 - Juan Manuel Perez-Mato  
Advanced studies of modulated structures  
Two more advanced (3+1)d examples

Lecture 4 - Olivier Gourdon  
Using incommensurate tools to investigate families of commensurate compounds

[1] [www-xray.fzu.cz/jana](http://www-xray.fzu.cz/jana)

[2] [superspace.epfl.ch/superflip](http://superspace.epfl.ch/superflip)

## **WK.02 Handling Twinning in Macromolecular Crystallography**

**George Sheldrick, Garib Murshudov, Peter Zwart, Presiding  
Conference B&C**

Twinning is a frequent problem in macromolecular crystallography that can easily be misunderstood and even lead to panic reactions. The aim of this workshop is to provide an understanding of twinning in a macromolecular context, and to show how one can often obtain entirely satisfactory and publishable structures despite twinning. Although small molecule crystallographers routinely determine twinned structures, this workshop is particularly timely because the latest versions of REFMAC and PHENIX\_REFINE now include facilities for refining twinned structures of macromolecules.

The morning lecture sessions will cover the principles of the detection, solution and refinement of twinned structures. In the afternoon there will be three parallel program demonstrations and discussions in small groups but participants may also work on their own data with expert assistance using laptops. Poster boards will be provided for participants to show their problem structures, solved or unsolved. The posters are intended to provide a focus for discussions in small groups.

8:30-9:05	Introduction to twinning. Regine Herbst-Irmer
9:05-9:40	Detection of twins. Todd Yeates
9:40-10:15	Twins and the phase problem. Zbigniew Dauter
10:15-10:45	Coffee Break
10:45-11:20	Processing non-merohedral twins and refinement with SHELX. George Sheldrick
11:20-11:55	Twin refinement with REFMAC. Garib Murshudov
11:55-12:30	Twin refinement with PHENIX_REFINE. Peter Zwart
12:30-14:00	Lunch and discussion
14:00-14:45	Computer demo I
14:45-15:30	Computer demo II
15:30-16:00	Coffee Break
16:00-16:45	Computer demo III
16:45-17:15	Further discussions at posters
17:15-17:30	Summing Up. Herb Klei

# SUNDAY, JULY 26

Registration Desk.....	07:30am .....	Grand Ballroom Foyer
Speaker Ready Room.....	07:30am .....	Conference C
Council Meeting Room.....	07:30am .....	Conference H
Accompanying Members Breakfast.....	09:00am .....	Carleton
Exhibit Show.....	10:00am .....	Sheraton/Osgoode Hall

## Opening Ceremony

**07:45am**                      **Grand Ballroom West**  
**Bob Von Dreele, ACA President, Presiding**

## SP.01 2009 Warren Award

**B. Von Dreele, Presiding**  
**Grand Ballroom West**

**08:00-08:10** Presentation of award to Chih-Lin Chang by Bob Von Dreele, ACA President.

**08:10-08:55**                      **SP.01.01**  
Coherent Dynamical Interaction in X-ray Multiple Diffraction and Crystal Cavity Resonance. Shih-Lin Chang.

## 01.01 Exciting Structures

**L. Kovari, Z. Yang, Presiding**  
**Grand Ballroom West**

**09:00-09:30**                      **01.01.01**  
The  $2.35 \approx$  Structure of *M. tuberculosis* NadE: Regulation of Active Site Coupling in Glutamine-dependent NAD<sup>+</sup> Synthetase. Nicole LaRonde-LeBlanc, Melissa Resto, Barbara Gerratana.

**09:30-10:00**                      **01.01.02**  
Crystal Structure and Association Behavior of the GluR2 Amino Terminal Domain. Rongsheng Jin, Satinder Singh, Shenyan Gu, Hiroyasu Furukawa, Alexander Sobolevsky, Jie Zhou, Yan Jin, Eric Gouaux.

**10:00-10:30**                      Coffee Break.

**10:30-11:00**                      **01.01.03**  
Structural Insight into the Essential Subunit Contact of the Influenza Virus RNA Polymerase. Sam-Yong Park, Eiji Obayashi, Hisashi Yoshida, Jeremy R. H. Tame, Atsushi Kawaguchi, Kyosuke Nagata.

**11:00-11:30**                      **01.01.04**  
The Structures of the G Protein Coupled Receptors: Implications for Signalling and Pharmacology. Gebhard Schertler.

**11:30-12:00**                      **01.01.05**  
Structural Basis of Recruitment of a Translesion DNA Polymerase to Sliding Clamp PCNA. Hong Ling, Guangxin Xing. Kevin Kirouac, Shin Yoon Jung, Bell Stephen.

## 02.01 General Interest I

**B. Noll, Presiding**  
**Grand Ballroom Centre**

### Revised schedule for 02.01

**09:00-09:20**                      **02.01.07**  
Rationalizing the Unusual Geometry in Heavy Alkaline Earth Metal Acetylides. Karin Ruhlandt-Senge, Marites Guino-o, Jacob Alexander, Ulrich Englisch, Hakon Hope.

**09:20-09:40**                      **02.01.02**  
Structural Analyses and Chemical Biology - Targeting the Kinetome of Apicomplexan parasites. Amy K. Wernimont, Wei Qiu, Mehrnaz Amani, Jennifer Artz, Yu-Hui Lin, Patrick Finerty, Martin Indarte, Masoud Vedadi, Matthieu Schapiro, Ray Hui.

**09:40-10:00**                      **02.01.03**  
Mutations and Polymorphism in Disease-related Proteins and their Effect on Protein Structure and Function. Seungjoo Lee, Vivien Yee.

**10:00-10:30**                      Coffee Break.

**10:30-10:45**                      **02.01.04**  
Pyrithyldion and Isopropylphenazone: Crystal Structures of their Polymorphs and their 1:1 Cocrystal. Andreas Lemmerer, Joel Bernstein, Volker Kahlenberg, Daniel Tobbens, Ulrich Griesser.

**10:50-11:10**                      **02.01.05**  
Structural Studies of S/Se Containing Neutral Radicals. Craig Robertson, Michael Probert, Judith Howard, Richard Oakley.

Film Presentation "Naturally Obsessed" .....	12:00pm .....	Conference B
Young Scientist SIG Meeting .....	01:00pm .....	Grand Ballroom Alley
President's Reception (invitation only) .....	04:30pm .....	Conference H
Poster Session P-S .....	05:30pm .....	Sheraton/Osgoode Hall
Young Scientist Mixer (ticket required) .....	08:00pm .....	Waterfall Garden/Sheraton

**11:10-11:30**                      **02.01.06**  
Two-photon Photodimerization Kinetics of the Single-crystal to Single-crystal Transformation of alpha-trans-cinnamic Acid to alpha-truxillic Acid. Jason Benedict, Philip Coppens.

**11:30-11:50**                      **02.01.09**  
Structure-Based Design of Farnesyl Pyrophosphate Synthase Inhibitors — Is Structure Most Important?. Bobby Barnett, Frank Ebetino, Richard Walter, Xhidao Xia, Artem Evedokimov, Matthew Pokross, Marlene Mekel, James Dunford, Graham Russell.

## 06.01 Supramolecular Chemistry

**C. Aakeroy, Presiding**  
**Grand Ballroom East**

**09:00-09:40**                      **06.01.01**  
Additive Induced Polymorphism. Gautam R. Desiraju.

**09:40-10:00**                      **06.01.02**  
Supramolecular Crystals by Hydrogen Bonding / Van der Waals Assembly of Non-self-complementary Molecules. Dmitriy V. Soldatov.

**10:00-10:30**                      Coffee Break.

**10:30-11:10**                      **06.01.03**  
Dynamic Porous Crystalline Materials Inspired By Halogen Bonding. Pierangelo Metrangolo, Yvan Carcenac, Manu Lahtinen, Tullio Pilati, Kari Rissanen, Ashvani Vij, Giuseppe Resnati.

**11:10-11:30**                      **06.01.04**  
A Template-directed Cross [2+2] Photoaddition of Olefins in a Three-component Solid Solution. Dejan-Kresimir Bucar, Leonard R. MacGillivray.

**11:30-11:50**                      **06.01.05**  
Single-Crystal to Single-Crystal Photochemistry in Supramolecular Systems. Menahem Kaftory, Tali Lavy, Irena Zouev, Marina Telzhensky, Den-Ke Cao, Gilad Golden, Mark Botoshansky.

*session continues after lunch at 01:30*

## 06.02 Energy Related Materials

**J. Hodges, Presiding**  
**Grand Ballroom Alley**

**09:00-09:30**                      **06.02.01**  
Application of the Pair-Distribution-Function Method to *in-situ* Studies in Catalysis. Peter Chupas, Karena Chapman.

**09:30-10:00**                      **06.02.02**  
Crystal Structures of  $M_nB_{12}H_{12}$  ( $n=1,2$ ) Compounds — Possible Intermediate Species in the Decomposition of  $M_n(BH_4)_2$ . Jae-Hyuk Her, Vitalie Stavila, Muhammed Yousufuddin, Wei Zhou, Satish Jalilatsgi, Ewa Ronnebro, Terrence Udovic.

**10:00-10:30**                      Coffee Break.

**10:30-11:00**                      **06.02.03**  
Structure and Characterization of Two Novel Aluminum Borohydride Amines. Antonio M. dos Santos, Claudia J. Rawn, Jianming Bai, Douglas A. Knight, Gilbert M. Brown.

**11:00-11:20**                      **06.02.04**  
*In-situ* XRD Investigations of the Solid—State Synthesis of Thermoelectric Cobalt Oxides. Haiyan Chen, Jianming Bai, Trevor Tyson.

**11:20-11:40**                      **06.02.05**  
Multi-Phase Behavior in Coordination

# SUNDAY, JULY 26

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Framework Materials at High Pressure. Karena Chapman, Gregory Halder, Peter Chupas.

**11:40-12:00** **06.02.06**  
Light-induced Phase Transition in VO<sub>2</sub> Thin Films. Huimin Liu, Sergiy Lysenko, Amando Rua, Felix Fernandez.

## **01.02 Vaccine Design**

**P. Kwong, I. Wilson, Presiding**  
**Grand Ballroom West**

**01:30-02:00** **01.02.01**  
Recognition of Influenza Virus by Broadly Neutralizing Antibodies: Implications for Vaccine Design. Ian Wilson, Damian Ekiert, Xueyong Zhu.

**02:00-02:30** **01.02.02**  
Challenges, Confusion, and Creativity in the Structure-based Design of Peptide Vaccines Based on Cellular immunity. Brian Baker.

**02:30-03:00** **01.02.03**  
Structure-based Design of a Composite Factor H Binding Protein as a Universal Vaccine for *Meningococcus B*. Rino Rappuoli.

**03:00-03:30** Coffee Break.

**03:30-04:00** **01.02.04**  
Structure-based Engineering for Vaccines: Adenovirus Vector and HIV-1 Envelope Immunogen. Bing Chen, Dan Barouch.

**04:00-04:30** **01.02.05**  
Computational Design of Immunogens to 'Re-elicite' Neutralizing Antibodies. William Schief.

**04:30-05:00** **01.02.06**  
Toward an Effective HIV-1 Vaccine: Structure-Assisted Immunogen Design of the HIV-1 Env. Peter Kwong.

## **06.01 Supramolecular Chemistry**

**C. Aakeroy, Presiding**  
**Grand Ballroom East**

**01:30-02:10** **06.01.06**  
Engineering Crystals and Other Materials. James Wuest.

**02:10-02:30** **06.01.07**  
Host-guest Behavior and Structural Dynamics in Hydrogen-bonded Metal-organic Frameworks (H-MOFs). Alicia Beatty, Chun-Long Chen, Greg Hogan.

**02:30-02:45** **06.01.08**  
Can Co-crystals Improve Aqueous Solubility of Anti-cancer Drugs? Safiyyah Forbes, Christer Aakeroy, John Desper.

**02:45-03:00** **06.01.09**  
Pharmaceutical Co-Crystals: Synthesis and Characterization of Model Compounds. Heba Abourahma, Nicole Morozowich, Marcos Marti.

**03:00-03:30** Coffee Break.

**03:30-04:10** **06.01.10**  
Is Polymorphism an Anathema to Crystal Engineering? Joel Bernstein.

**04:10-04:30** **06.01.11**  
Towards Knowledge-based Design and Control of Pharmaceutical Crystal Forms. Colin R. Groom, Peter T. A. Galek, Peter A. Wood.

**04:30-04:50** **06.01.12**  
Are There Really any Reliable and Versatile Strategies for Co-crystal Synthesis out There? Christer Aakeroy.

*Session continues tomorrow at 01:30*



# MONDAY, JULY 27

Rigaku Fun Run.....	06:30am.....	Meet in hotel lobby
Registration Desk.....	07:30am.....	Grand Ballroom Foyer
Speaker Ready Room.....	07:30am.....	Conference C
Council Meeting Room.....	07:30am.....	Conference H
Exhibit Show.....	10:00am.....	Sheraton/Osgoode Hall
Rigaku Lunch & Learn.....	12:00pm.....	Essex Ballroom
Brucker Lunch (Invitation only).....	12:00pm.....	Civic Ballroom
BioMac SIG Meeting.....	05:00pm.....	Grand Ballroom West

## SP.02 Etter Early Career Award

R. Huether, Presiding  
Grand Ballroom West

Presentation of award to Svilen Bobev by Bob Von Dreele, ACA President.

**08:00-08:55** **SP.02.01**  
**Rare-Earth Intermetallics - How Far Does One Need to Go Searching for New Structures and Properties.** Svilen Bobev.

**09:00-09:15** **SP.02.02**  
Investigating the Structural Basis of a Novel Domain Implicated in pre-mRNA Recognition by a Splicing Factor Complex. Ankit Gupta, Clara L. Kielkopf.

**09:15-09:30** **SP.02.03**  
Novel van der Waals Solid Phases in the Methane-Nitrogen Binary System. Catherine Aldous, Serge Desgreniers.

**09:30-09:45** **SP.02.04**  
Structural Analysis of Engineered N-acetyl-D-neuraminic Acid Lyase. Ivan Campeotto\*, Arwen Pearson, Adam Nelson, Alan Berry, Simon E. V. Phillips. \*Young Scientist SIG Student Lecturer Awardee

**09:45-10:00** **SP.02.05**  
Average Structure of a Modulated Profilin: Actin Crystal. Jason Porta, Jeff Lovelace, Gloria Borgstahl.

**10:00-10:30** **Coffee Break.**

**10:30-10:50** **SP.02.06**  
Navigating the Difficulties of Crystal Structure Determination of Endohedral Metalofullerenes. Brandon Mercado, Christine Beavers, Marilyn Olmstead, Manuel Chaur, Keith Walker, Brian Holloway, Luis Echegoyen, Alan Balch.

**10:50-11:10** **SP.02.07**  
Guest Inclusion in Pillared Hydrogen Bonded Metal-Organic Frameworks (HMOFs). Greg A. Hogan, Alicia M. Beatty.

**11:10-11:30** **SP.02.08**  
X-ray Crystal Structure of Epi-isozizaene Synthase from *Streptomyces coelicolor*. Julie Aaron, Cristina Virgilio, Xin Lin, David Cane, David Christianson.

**11:30-11:45** **SP.02.09**  
Biochemical and Structural Studies of CpxP, Inhibitor of the Cpx Envelope Stress Response in *Escherichia coli*. Gina Thede, David Arthur, Ross Edwards, Daelynn Buelow, Tracy Raivio, Mark Glover.

**11:45-12:00** **SP.02.10**  
Self-assembling Reversible Hydrogen and Halogen-bonded CavitanDs. Arbin Rajbanshi, Christer Aakeroy, John Desper.

General Interest Meeting .....	05:00pm .....	Grand Ballroom Centre
Neutron, Powder, Materials Joint SIG Meeting.....	05:00pm .....	Grand Ballroom East
Industrial SIG Meeting.....	05:00pm .....	Grand Ballroom Alley
Poster Session P-M.....	05:30pm .....	Sheraton Hall/Osgoode
06.06 Would You Publish This? .....	07:00pm .....	Grand Ballroom East
Rayonix Jazz Night (pick up at Rayonix booth) .....	07:30pm .....	The REX
Mentor/Mentee Dinner (ticket required) .....	08:00pm .....	Forestview Chinese Restaurant

**TR.01 Transactions Symposium: Phase Transitions**

**R.J. Angel, I. Swainson, Presiding**  
**Grand Ballroom East**

**09:00-09:15** Introduction. R.J. Angel.

**09:15-09:45** **TR.01.01**  
 High Pressure Phase Transitions In Molecular Crystals. Simon Parsons.

**09:45-10:00** **TR.01.02**  
 Phase Behavior of Water Inside Protein Crystals. Chae Un Kim, Irina Kriksunov, William A. Miller, Doletha M.E. Szebenyi, Sol M. Gruner.

**10:00-10:30** Coffee Break.

**10:30-10:45** **TR.01.03**  
 Structural Properties of the Continuous, Reversible Order Disorder Process of the Cu(I) Ions in  $[(C_6H_5)_3PCH_3]Cu_3BR_4$ . Roger Willett, Salim Haddad, Brendan Twamley.

**10:45-11:15** **TR.01.04**  
 Nature's Basis for Parameterizing Structural Phase Transitions. Branton Campbell, Harold T. Stokes, John S.O. Evans, Francesca Perselli, Sean C. Kerman, Kiran K. Satyavarapu.

**11:30-12:00** **TR.01.05**  
 Symmetry Aspects of Structural Phase Transitions: Ferroics and Multiferroics. J. Manuel Perez-Mato.

*session continues after lunch at 01:30*

**01.03 Crystallization Methods**

**A. Edwards, A. McPherson**  
**Grand Ballroom Centre**

**09:00-09:30** **01.03.01**  
 Submit Your Sequence and We Deliver: Remarks of a Fed-up Crystallographer. Bernhard Rupp.

**09:30-09:45** **01.03.02**  
 A Microscopic View of Protein Crystallization. Zygmunt Derewenda, Marcin Cieslik, David Cooper.

**09:45-10:00** **01.03.03**  
 Elucidating the Chemical and Physical Properties Controlling Protein Expression and Crystallization. Nicholson Price II, Yang Chen, Samuel Handelman, Philip Manor, Rajesh Nair, Jinfeng Liu, George DeTitta, Burkhard Rost, Gaetano Montelione, John Hunt.

**10:00-10:30** Coffee Break.

**10:30-10:45** **01.03.04**  
*In situ* Proteolysis to Generate Crystals for Structure Determination: An Update. Aiping Dong, Amy Wernimont, Xiaohui Xu, Alexei Savchenko, Andrzej Joachimiak, Cheryl Arrowsmith, Alexey Bochkarev, Aled Edwards, Midwest Consortium for Structural Genomics, Structural Genomics Consortium.

**10:45-11:00** **01.03.05**  
 Diffraction Study of Protein Crystals Grown in Loops and Micromounts. Irimpan Mathews, Michael Berger, Johannes Decker.

**11:00-11:15** **01.03.06**  
 A Different Take on Crystallization: The Rational Design of a Self-Assembled Three-Dimensional DNA Crystal. Nadrian Seeman,

# MONDAY, JULY 27

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Jianping Zheng, Jens Birktoft, Ruojie Sha, Tong Wang, Pamela Constantinou, Yi Chen, Chengde Mao, Stephen Ginnell.

**11:15-11:30** **01.03.07**  
Directed Crystallization on 2D Monolayer Templates. Ilana G. Goldberg, Linsey E. Roeker, David Black, Jennifer A. Swift.

**11:30-11:45** **01.03.08**  
Towards Efficient Crystallization Screening Using UV Fluorescence Imaging. Jian Xu, Craig Sterling, Michael Willis.

**11:45-12:00** **01.03.09**  
Macromolecule-peptide Fusions as Tools for Crystallization of Glycopeptide Antibiotics. Nicoleta Economou, Stephen D. Weeks, Kimberly C. Grasty, Virginie Nahoum, Patrick J. Loll.

## **06.04 Diffraction Studies & Mechanical Properties of Engineering Materials**

**R. Rogge, Presiding**  
**Grand Ballroom Alley**

**09:00-09:30** **06.04.01**  
Monitoring the Development of the Texture and Phase of Shape Memory Alloys using *in-situ* Neutron Diffraction During Deformation and Thermal Cycling. Donald Brown, Thomas Sisneros, Raj Vaidyanathan, Robert Field, Catherine Tupper.

**09:30-09:45** **06.04.02**  
Prevention of Strain Recovery in the Uranium 6 wt% Niobium Shape Memory Alloy. Catherine Tupper\*, Don Brown, Bjorn Clausen, Robert Field. \**Neutron Scattering SIG Student Lecturer Awardee*

**09:45-10:00** **06.04.03**  
Neutron Diffraction Studies of Phase Composition of UMo-Al Dispersion Fuels Subjected to Partial Burnup. Ian P. Swainson, K.T. Conlon, D. Sears, R. Rogge, L.M.D. Cranswick, R. Donabarger

**10:00-10:30** Coffee Break.

**10:30-11:00** **06.04.04**  
Tracking Diffraction Profile Evolution During Liquid Phase Sintering of Interacting Isomorphous Powder Blends. Dennis Turriff, Stephen Corbin, Lachlan Cranswick.

**11:00-11:15** **06.04.05**  
Microstructural and Crystallographic Study on Phase Stability of Tetragonal Zirconia Powders Prepared by Chemical Methods: XRD—FTIR Link. Diego Andres Campo Ceballos, Jorge Enrique Rodriguez Paez.

**11:15-11:30** **06.04.06**  
Trends in the Thermal Expansion Behaviour of  $AM_2(PO_4)_3$  NZP Type Structures [M = Sn, Ge; A = Li, Na, K, Rb, Cs, Ag, Cu]. David Billing, Roy Forbes.

**11:30-11:45** **06.04.07**  
Local Structure and its Relationship to the Physical Properties of Low and Negative Thermal Expansion Frameworks. Angus Wilkinson, Benjamin Greve, Andrew Jupe, Chad Ruschman, Mehmet Cetinkol, Kenneth Martin, Karena Chapman, Peter Chupas, Peter Lee.

## **TR.01 Transactions Symposium: Phase Transitions**

**R.J. Angel, I. Swainson, Presiding**  
**Grand Ballroom East**

**01:30-02:00** **TR.01.06**  
Advances in Automated Twin Data Processing in CrysAlisPro. Mathias Meyer.

**02:00-02:30** **TR.01.07**  
Modulated Phases and their Analysis with Jana2006. Michal Dusek, Vaclav Petricek.

**02:30-03:00** **TR.01.08**  
Data Collection and Processing of Incommensurately Modulated Structures at Varying Temperatures. Michael Ruf, Garold Bryant, Bruce Noll, Joerg Kaercher.

**03:00-03:30** Coffee Break.

**03:30-04:00** **TR.01.09**

Phase Transitions in Microporous Materials. G. Diego Gatta.

**04:00-04:30** **TR.01.10**

Using the Bond Valence Model to Analyse Structural Chemistry Across Phase Boundaries. David Brown.

**04:30-05:00** **TR.01.11**

Local Structure and Crystallographic Phase Transitions. Thomas Proffen.

## **06.01 Supramolecular Chemistry**

**C. Aakeroy, Gary Enright, Presiding  
Grand Ballroom Centre**

**01:30-01:45** **06.01.13**

Uranyl-bound Halogens as Hydrogen-bond Acceptors: Applying Supramolecular Chemistry to the Actinides. Nicholas Deifel, Christopher Cahill.

**01:45-02:00** **06.01.14**

Toward Porous Hydrogen-bonded Metal Organic Frameworks (HMOFs). Onome Ugono, Alicia Beatty.

**02:00-02:15** **06.01.15**

Building Porous Solids with Porphyrins: Strategic Routes for New Materials. Wonyoung Choe.

**02:15-02:30** **06.01.16**

Metal-metal and Metal-grid Interactions Leading to Extended Structural Motifs: A Step Towards Functional Molecular Platforms. Louise Dawe, Victoria Milway, Laurence Thompson.

**02:30-02:45** **06.01.17**

Design of Porous Metal-organic Frameworks Utilizing 4-(imidazolyl)benzoic Acids. Moqing Hu, Lisa Lee, Timothy Lawton, John MacDonald.

**02:45-03:00** **06.01.18**

Phase- and Structure-Directing Factors in Cobalt Orotate Hydrates. Larry R. Falvello, Pablo Guerra, Gema Martinez, Nuha Mushale, Milaros Tomas.

**03:00-03:30** Coffee Break.

**03:30-03:45** **06.01.19**

Supramolecular Dating: Who Will Go With Whom? Prashant Chopade, Christer Aakeroy, John Desper.

**03:45-04:00** **06.01.20**

Predicted and Unpredicted Cocrystals of m-Hydroxybenzoic Acid and Acridine. Daniel Adsmund, Joel Bernstein, Radion Vainer.

**04:00-04:15** **06.01.21**

Quantification of Uric Acid Single Crystal Adhesion Forces by Atomic Force Microscopy. Janeth Presores, Jennifer A. Swift.

**04:15-04:30** **06.01.22**

Supramolecular Structures in the Systems:  $\alpha$ -cyclodextrin/camphor/alcohol / water and  $\beta$ -cyclodextrin/cis-decaline/dimethylformamide. Janusz Lipkowski.

**04:30-04:45** **06.01.23**

The Formation of a Two-Component Salt by Both Solution and Non-Solution Techniques. Claire Cook, Roger Davey, Simon Black.

**04:45-05:00** **06.01.24**

Intermolecular Interactions in Benzene- and Pyridine-Solvated Crystals. Raymond E. Davis, Hernan Oswaldo Aldas-Palacios.

## **06.05 Structure-based Drug Design**

**E. Arnold, D. McRee, Presiding  
Grand Ballroom West**

**01:30-01:35** Introduction. Duncan McRee.

**01:35-02:05** **06.05.01**

Drug Design by Fragment Screening for

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HIV-1 Reverse Transcriptase. Joseph Bauman, Disha Patel, Chhaya Dharia, Sameer Ahmed, Marc Fromer, Arthur Clark, J. Thomas Eck, William Ho, Eddy Arnold.

**02:05-02:30** **06.05.02**  
From Fragment to Candidate. Pamela Williams.

**02:30-03:00** **06.05.03**  
Antivirals and Drug Resistance. Peter Colman.

**03:00-03:30** Coffee Break.

**03:30-04:00** **06.05.04**  
Ligand Efficiency Indices for a More Effective Structure-Based Drug Discovery. Celerino Abad-Zapatero.

**04:00-04:30** **06.05.05**  
Structure Based Approach to the Identification of a Small Molecule Protein-Protein Interaction Inhibitor. Alexandru Ghetu, Gil Prive.

**04:30-05:00** **06.05.06**  
Attenuating  $\beta$ -lactam Antibiotic Resistance in Gram-negative Pathogens: Targeting the AmpC  $\beta$ -lactamase Induction Pathway. B.L. Mark, D. J. Vocadlo, M. Balcewich, A.

## 06.19 Membranes and Associated Proteins

**T. Weiss, Presiding**  
**Grand Ballroom Alley**

**01:30-02:00** **06.19.01**  
Interaction of Cholesterol and Phospholipids in Cell Membranes. David Gidalevitz.

**02:00-02:30** **06.19.02**  
Understanding Membrane Protein Crystallization in the Bicelle System. Ursula Perez-Salas, Ann Carol Kimble-Hill, Michael Schultz, Andrea Hamill, Lionel Porcar, Paul Butler.

**02:30-03:00** **06.19.03**  
Crystal Structure of LPD-12: A Self-assembling Lipopeptide Detergent at 1.20  $\text{\AA}$ . Gil Prive, Dona Ho, Neil Pomroy, Jose Cuesta-Seijo, Hamed Ghanei.

**03:00-03:30** Coffee Break.

**03:30-04:00** **06.19.04**  
The Structure of a Cytolytic  $\alpha$ -helical Toxin Pore Reveals its Assembly Mechanism. Marcus Mueller, Ulla Grauschopf, Timm Maier, Rudi Glockshuber, Nenad Ban.

**04:00-04:30** **06.19.05**  
Crystallographic Structure of Xanthorhodopsin, the Light-driven Proton Pump with a Dual Chromophore. Hartmut Luecke.

**04:30-05:00** **06.19.06**  
Crystal Structure of RPE65, the Retinoid Isomerase of the Visual Cycle. Philip Kiser, Marcin Golczak, David Lodowski, Mark Chance, Krzysztof Palczewski.

Asgarali, K. A. Stubbs.

**EVENING SESSION****06.06 Would You Publish This?****C. Slebodnick, Presiding****Grand Ballroom East 07:00-09:00****06.06.01**

Pyrazine Bridged Ruthenium(III)-Platinum(II) Complexes: The Good, the Bad, and the Ugly. Joseph M. Tanski, C.M. Anderson.

**06.06.02**

Disorder in Pyridyl Based Cryptands Complexed with Bipyridinium Salts. Carla Slebodnick, Adam M. -P. Pederson, Harry W. Gibson.

**06.06.03**

Barely Publishable (?) Porphyrin Structures. Frank R. Fronczek.

**06.06.04**

Trials and Tribulations in Solving Metal-Organic Framework Problems: Confessions of a MOF Novice. Amy Sarjeant.

**06.06.05**

Crystal Structure of a Weakly Diffracting Chiral Organic Molecule. Gary D. Enright.

**06.06.06**

Isosteric Quasiracemate or Not? Where's the Border? Gregory M. Ferrence, Kate L. Edler, Lindsay R. Hedge, Adam D. Beitelman, Matthias Zeller, Shawn R. Hitchcock.

**06.06.07**

Refinement Issues With Non-centrosymmetric Structures With Pseudo-inversion Symmetry. Victor Young.

Discussion to follow presentations.

**2009 Margaret C. Etter Student Lecturer Awards**

Each Special Interest Group (SIG) has the opportunity to select one student to receive an award and to present a lecture in one of the sessions organized by that SIG. 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 this year's winners:**

BioMac .....	Alaji Bah .....	Washington U., Sch. of Medicine .....	06.20.03
Materials Science .....	Jinsheng Wen .....	Brookhaven National Lab .....	06.18.03
Neutron Scattering .....	Catherine Tupper .....	Los Alamos National Lab .....	06.04.02
Powder Diffraction .....	Matt Beekman .....	Univ. of South Florida .....	06.15.04
Service Cr .....	Partha P. Das .....	Univ. of Zurich .....	06.08.04
Small Angle Scattering .....	Peter Gin .....	Stony Brook Univ. ....	04.01.04
Synchrotron Radiation .....	Jesse Smith .....	Univ. of Ottawa .....	06.10.07
Young Scientist .....	Ivan Campeotto .....	Univ. of Leeds .....	SP02.04

Registration Desk.....	07:30am .....	Grand Ballroom Foyer
Speaker Ready Room.....	07:30am .....	Conference C
Council Meeting Room.....	07:30am .....	Conference H
Exhibit Show.....	10:00am .....	Sheraton/Osgoode Hall
Canadian Div. Meeting.....	12:00pm.....	Grand Ballroom Centre
IUCr Commission on Journals.....	12:00pm.....	Simcoe

## SP.03 Plenary Lecture

**W. Duax, Presiding**  
**Grand Ballroom West**

**08:00-08:10** Introduction. Bill Duax,  
 ACA CEO.

**08:10-08:55** **SP.03.01**  
 Celebrating Crystallography. Ted Baker.

## 06.07 Superconducting Materials

**J.F. Mitchell, Presiding**  
**Grand Ballroom Centre**

**09:00-09:30** **06.07.01**  
 Superconductivity, Crystal Structures and Phase Transitions of Layered Iron Arsenides. Dirk Johrendt, Marianne Rotter, Markus Tegel.

**09:30-10:00** **06.07.02**  
 Key Role of Iron-Magnetism in High-Temperature Fe-Pnictide Superconductors. Taner Yildirim.

**10:00-10:30** Coffee Break.

**10:30-10:50** **06.07.03**  
 Similarities Between Structural Distortions Induced by Pressure and Chemical Doping in Superconducting BaFe<sub>2</sub>As<sub>2</sub>. Simon Kimber, Dimitri Argyriou.

**10:50-11:10** **06.07.04**  
 Pressure-Induced Effects on the Structure of the FeSe Superconductor. Jasmine Millican, Daniel Phelan, Evan L. Thomas, Juscelino B. Leão, Elisabeth Carpenter.

**11:10-11:30** **06.07.05**  
 Facilities for Superconductor Vortex-lattice Crystallography at the HFIR Research Reactor. Kenneth C. Littrell, Katherine M. Bailey,

Christopher M. Redmon, David A. Reass, Mano Sanchez, Jonathan R. Smith.

**11:30-12:00** **06.07.06**  
 Synthesis, Crystal Structure and Physical Properties of Cobalt Oxyhydrate Superconductors. Eiji Takayama-Muromachi.

## 06.08 Problem Structures: Solution and Refinement of Particularly Difficult Small Molecules Structures

**R.J. Staples, Presiding**  
**Grand Ballroom Alley**

**09:00-09:20** **06.08.01**  
 Might as Well Face It, I'm Addicted to Flux: The Joys of Synchrotron Chemical Crystallography. Christine M. Beavers, Marilyn M. Olmstead, Brandon Q. Mercado.

**09:20-09:40** **06.08.02**  
 Diffraction Pattern and Incommensurately Modulated Superstructures of BaM<sub>1-x</sub>Te<sub>2</sub> (M = Cu, Ag, Au; x ≈ 0.33). Christian Graf, Yanjie Cui, Mayasree Ootil, Assoud Abdeljalil, Kleinke Holger.

**09:40-10:00** **06.08.03**  
 For a Commensurately Modulated Structure, Different Index Conditions can see Different Average Structures. A. David Rae.

**10:00-10:30** Coffee Break.

**10:30-10:45** **06.08.04**  
 α-NaLuF<sub>4</sub>: A Structure for All Seasons. Partha P. Das\*, Lukas Palatinus, Hans-Beat Buerger, Anthony Linden. \*Service Crystallography SIG Student Lecturer Awardee

Film Presentation "Naturally Obsessed" .....	12:00pm .....	Conference B
Service SIG Meeting .....	12:00pm .....	Grand Ballroom West
Synchrotron SIG Meeting .....	12:00pm .....	Grand Ballroom East
SAS/Fiber Diffraction Joint SIG Meeting .....	05:00pm .....	Grand Ballroom East
Small Mol SIG Meeting .....	05:00pm .....	Grand Ballroom West
Poster Session P-T .....	05:30pm .....	Sheraton/Osgoode Hall

**10:45-11:10** **06.08.05**  
 Are Modulated and Composite Structures Still Difficult Ones? Vaclav Petricek, Michal Dusek.

**11:10-11:35** **06.08.06**  
 Looking for Unresolved Symmetry in High Z' Crystal Structures. Victor Young.

**11:35-12:00** **06.08.07**  
 The Application of a Molecular Replacement Approach to the Refinement of a Copper Nanoball Complex from Low Resolution Data. Charles Campana, Christopher Waddling, Randy Larsen, Gregory McManus, John Perry, Edwin Rivera-Otero, Michael Zaworotko.

## **06.09 Refinement (Computational)**

**E. Collins, P. Horanyi, Presiding**  
**Grand Ballroom West**

**09:00-09:20** **06.09.01**  
 REFMAC: A Program for Macromolecular Crystal Structure Refinement. Garib Murshudov, Pavol Skubak, Alexei Vagin, Navraj Panu, Fei Long, Andrey Lebedev.

**09:20-09:40** **06.09.02**  
 Recent Enhancements in the Structure Refinement Capabilities of BUSTER-TNT. G. Bri-cogne, M. Brandl, C. Flensburg, P.A. Keller, W. Paciorek, O.S. Smart, C. Vornrhein, T.O. Womack.

**09:40-10:00** **06.09.03**  
 Automated Structure Determination with Phe-nix. Paul Adams, Pavel Afonine, Nat Echols, Ralf Grosse-Kunstleve, Nigel Moriarty, Peter Zwart.

**10:00-10:30** Coffee Break.

**10:30-11:00** **06.09.04**  
 Structure Refinement at Low Resolution. Axel Brunger, Gunnar Schroeder, Michael Levitt.

**11:00-11:20** **06.09.05**  
 Real and Reciprocal Space Refinement in Ser-vice of NCS in Single and Multiple Crystal Form Structure Determination. Dusan Turk.

**11:20-11:40** **06.09.06**  
 Refinement with Local Structure Similarity Restraints (LSSR) Enables Exploitation of In-formation from Related Structures and Facili-tates use of NCS. Oliver Smart, Maria Brandl, Claus Flensburg, Peter Keller, Wlodek Pacio-rek, Clemens Vornrhein, Thomas Womack, Gerard Bricogne.

**11:40-12:00** **06.09.07**  
 SHAKERR: A Tool for Evaluation of the Precision of Crystal Structure Model. Edwin Pozharski, Timothy D. Fenn, Mark A. Wilson.

## **06.10 Instrumentation: Sources, Optics, Robotics and Detectors**

**M. Allaire, C. Ogata, Presiding**  
**Grand Ballroom East**

**09:00-09:30** **06.10.01**  
 First Science from the Compact Light Source. Ronald Ruth, Jeffrey Rifkin, Loewen Roderick.

**09:30-10:00** **06.10.02**  
 Single Molecule Imaging Possibilities at the Linac Coherent Light Source. Sebastien Boutet.

**10:00-10:30** Coffee Break.

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**10:30-11:00** **06.10.03**  
New Instrumentation at the SLS PX -  
Beamlines. Clemens Schulze-Briese, Rou-  
ven Bingel-Erlenmeyer, Martin Fuchs, Jose  
Gabardino, Wayne Gletting, Vincent Olieric,  
Robin Owen, Ezequiel Panapucci, Takashi  
Tomizaki, Meitian Wang.

**11:00-11:30** **06.10.04**  
CMCF2 (08B1) High-Throughput Mac-  
romolecular Crystallography Beamline at  
the Canadian Light Source. Michel Fodje,  
Pawel Grochulski, Kevin Anderson, Natalie  
Strynadka.

**11:30-12:00** **06.10.05**  
Commissioning Report from the X9 X-ray  
Scattering Beamline at NSLS. Lin Yang.

*session continues after lunch at 01:30*

**01:30-02:00** **06.10.06**  
Opportunities for Life Sciences at NSLS-II.  
Wayne Hendrickson, Lisa M. Miller.

**02:00-02:15** **06.10.07**  
Exploiting Area Detectors to Reduce Compton  
Scattering via Energy Selection and to  
Measure Beamline Polarization at Syn-  
chrotron Radiation Facilities. Jesse Smith\*,  
Serge Desgreniers. \**Synchrotron Radiation*  
*SIG Student Lecturer Awardee*

**02:15-02:35** **06.10.08**  
XAMPS: A Monolithic Active-matrix Sili-  
con X-ray Detector for Protein Crystallogra-  
phy. Gabriella Carini, Angelo Dragone, Wei  
Chen, Jack Fried, Jean Jakoncic, Anthony  
Kuczewski, Zheng Li, Joseph Mead, Pavel  
Rehak, Peter Siddons.

**02:35-03:00** **06.10.09**  
G-Rob, a 6-axis Robotic Arm Based Auto-  
mated System for Crystallography. Jean-  
Luc Ferrer, Jacques Joly, Xavier Vernede,  
Philippe Charrault, Michel Pirrochi, Florian  
Bouis, Joly Quilez, Gael Pages.

**03:00-03:30** Coffee Break.

**03:00-03:30** **06.10.10**  
Microdiffraction Studies at the ESRF-ID13  
Beamline. Christian Riekel.

**04:00-04:30** **06.10.11**  
Probing Radiation Damage in Protein Crys-  
tals with a 1-micron X-ray Beam. Rus-  
lan Sanishvili, Derek Yoder, Sudhirbabu  
Pothineni, Janet Smith, Gerd Rosenbaum,  
Shenglan Xu, Oleg Makarov, Sergey Stepa-  
nov, Stefan Vogt, Robert Fischetti.

**04:30-05:00** **06.10.12**  
Picosecond Time-resolved Science at Bio-  
CARS. Timothy Graber, R. W. Henning, I.  
Kosheleva, Z. Ren, V. Srajer, K. Moffat, H-S  
Cho, N. Dashdorj, F. Schotte, P. Anfinrud.

## **06.11 Cooperative Phenomena in Magnetic Materials**

**O. Garlea, Presiding**  
**Grand Ballroom Centre**

**01:30-02:00** **06.11.01**  
Neutron Scattering from Geometrically  
Frustrated Pyrochlore Magnets. Bruce  
Gaulin.

**02:00-02:30** **06.11.02**  
Chiral Magnetic Order in Fe Based Langas-  
ites. Pierre Bordet, Karol Marty, Virginie  
Simonet, Eric Ressouche, Rafik Ballou,  
Celine Darie, Jakob Kljun, Olivier Isnard,  
Pascal Lejay.

**02:30-03:00** **06.11.03**  
Searching for Stripes in Short Range Charge  
and Spin Superstructures. Andrei Savici,  
Igor Zaliznyak, Genda Gu, Ross Erwin,  
Ying Chen, Hye Jung Kang.

**03:00-03:30** Coffee Break.

**03:30-04:00** **06.11.04**  
Uncharacteristic Phase Separation Trends  
with the Ionic Size in Cobaltites. Despina  
Louca, Juan Yu, Danniell Phelan.

**04:00-04:20** **06.11.05**  
Coexistence of Weak Ferromagnetism and Ferroelectricity in a High Pressure Form of  $\text{FeTiO}_3$ . John Mitchell, Tamas Varga, Venkataraman Gopalaran, Xianglin Ke, Amit Kumar, Peter Schiffer, Yanbin Wang.

**04:20-04:40** **06.11.06**  
Magnetic Structures of  $\text{NaLnMnWO}_6$  ( $\text{Ln}=\text{La}, \text{Nd}, \text{Tb}$ ) Perovskites. Graham King, Andrew Wills, Patrick Woodward.

**04:40-05:00** **06.11.07**  
Pressure-induced Sequential Reorientation of the Jahn-Teller Axis in a Magnetic Molecular Material. Gregory Halder, Karena Chapman, Jamie Manson, Hyunsoo Park, John Schlueter.

## 06.13 Large Small Molecules

**I. Guzei, Presiding**  
**Grand Ballroom West**

**01:30-01:55** **06.13.01**  
Direct Methods for Larger Structures. George M. Sheldrick.

**01:55-02:20** **06.13.02**  
SHELXL Refinement in the Realm of Large Small Molecules - Higher Fullerenes and a Small Protein - Observations and Methods. Marilyn Olmstead, Christine Beavers, Brandon Mercado, Hua Yang, James Nowick.

**02:20-02:40** **06.13.03**  
The  $1.4 \approx$  Crystal Structure of Ramoplanin, a Large Natural Product Antibiotic. Patrick Loll, James Hamburger, Amanda Hoertz, Amy Lee, Rachel Santuria, Dewey McCafferty.

**02:40-03:00** **06.13.04**  
Unambiguous Determination of Hydrogen Atom Positions - A Quantitative Comparison of X-ray, Neutron, and Joint Refinements of Rubredoxin. Anna Gardberg, Flora Meilleur, Kevin Weiss, Qiu Zhang, Matthew Blakeley, Dean Myles.

**03:00-03:30** Coffee Break.

**03:30-03:55** **06.13.05**  
High  $Z'$  Structures, Modulated and Not. Carolyn P. Brock.

**03:55-04:15** **06.13.06**  
Facilities for Structural Biology and Chemical Crystallography at Diamond Light Source. Michael Engel, E.J. Shotton.

**04:15-04:35** **06.13.07**  
The Application of Non-ambient Techniques to Small Molecule Single Crystal X-ray Diffraction. John Warren.

**04:35-05:00** **06.13.08**  
What is a Large Small Molecule to Powder Diffraction? Peter Stephens.

## 06.12 Professional Directions

**01:40-4:30**  
**R. Jackson, H. Klei, Presiding**  
**Grand Ballroom Alley**

The session will be a panel discussion involving participants who are engaged in a variety of crystallography-related careers. The panelists include individuals employed in academics, government, and industry. The aim is to give attendees an opportunity to learn about different professional avenues available to those with training in crystallography and to ask questions of the panelists.

*Panelists will be:*

Steve Ginell, SBC-CAT @Argonne Labs  
Jim Kaduk, INEOS Technologies  
Steven Sheriff, Bristol Myers-Squibb  
Charlotte Stern, Northwestern University  
Paul Swepston, Rigaku Americas  
Carrie Wilmot, U. of Minnesota  
Mark Wilson, U. of Nebraska-Lincoln

Registration Desk.....	07:30am .....	Grand Ballroom Foyer
Speaker Ready Room.....	07:30am .....	Confernece C
Council Meeting Room.....	07:30am .....	Conference H
Film: H.M. Hauptman, Ph.D., "Portrait of a Laureate" (WNED) 12:15pm.....		Conference B
Meet Dr. Hauptman, winner 1985 Nobel Prize in Chemistry, after the 30 minute film		

## SP.04 Plenary Lecture

**S. Larsen, Presiding**  
**Grand Ballroom West**

**08:00-08:10** Introduction. Sine Larsen, IUCr President.

**08:10-08:55** **SP.04.01**  
New Developments in X-ray Photocrystallography: From Hours to Microseconds and Beyond. Philip Coppens.

## 05.01 Cool Structures

**P. Mueller, Presiding**  
**Grand Ballroom Centre**

**09:00-09:30** **05.01.01**  
Experimental and Theoretical Determination of the Electron Density Distribution of  $\alpha,\alpha$ -Trehalose Dihydrate. Edwin Stevens, Michael Dowd, Glenn Johnson, Alfred French.

**09:30-10:00** **05.01.02**  
Direct Visualization of Hydrogen Behavior in Rare-Earth/Transition-Metal Hydride Clusters by SR Charge Density Study. Nobuhiro Mizuno, Takanori Shima, Zhaomin Hou, Masaki Takata.

**10:00-10:30** Coffee Break.

**10:30-11:00** **05.01.03**  
Polymorphism of a N-Benzoyl-Guanidine: 4-Methoxy -1-[4-methoxyanilino(phenylcarbonylimino)-methylamino]benzene. Hamilton Napolitano, Carlito Lariucci, Ademir Camarago, Silvio Cunha.

**11:00-11:30** **05.01.04**  
Adventures in Coordination Chemistry with Bad Ligands. Joseph Tanski, Tamila Shalunova, Greg Maier.

**11:30-12:00** **05.01.05**  
Is There any Real Bond Between Metal Atoms

in the Clusters  $[\text{Zn}_2(\eta^5\text{-C}_5\text{Me}_5)_2]$  and  $[\text{Ru}_3(\mu\text{-H})_2(\mu_3\text{-MeImCH})(\text{CO})_9]$ ? Juan Van der Maelen, Santiago García-Granda.

## 06.14 Diagnostics During Data Collection

**E. Bergmann, M. Fodje, Presiding**  
**Grand Ballroom West**

**09:00-09:20** **06.14.01**  
Discovering the Rules of Successful Protein Structure Determination with Simulated Diffraction Images. James Holton.

**09:20-09:40** **06.14.02**  
Signal-Based Data Collection: An Approach to Automated Data Collection Aimed at Increasing Structure Solution Success. John Rose, John Chrzas, Zheng-Qing Fu, James Fait, John Gonczy, Zhongmin Jin, Andrew Howard, Bi-Cheng Wang.

**09:40-10:00** **06.14.03**  
Phosphor-SAD Phasing as a General Tool for Solving Nucleic Acid Structure? Meitian Wang, Vincent Olieric, Eric Ennifar, Philippe Dumas, Clemens Schulze-Briese.

**10:00-10:30** Coffee Break.

**10:30-11:00** **06.14.04**  
Optimal Analysis of Highly Exposed Macromolecular Crystals. Zbyszek Otwinowski, Dominika Borek, Marcin Cymborowski, Wladek Minor.

**11:00-11:20** **06.14.05**  
Structural Insights into Terminal Double Bond Formation in the Curacin A Biosynthetic Pathway. Jennifer Gehret, Liangcai Gui, David H. Sherman, Janet L. Smith.

**11:20-11:40** **06.14.06**  
Use of Micro-focused Beamline in Solving

**All Member Business Meeting .....05:00pm.....Grand Ballroom West**  
**Annual Award Banquet** (ticket required)  
 Cash Bar .....06:30pm-07:30pm ..... Dominion Ballroom Foyer  
 Dinner.....07:30pm-10:30pm ..... Dominion Ballroom

the Crystal Structure of the Avian Thymic Hormone (ATH) in the Calcium Bound Form. Jonathan Schuermann, John Tanner, Michael Henzl.

Carbon Graphene and Nanotube Arrays with Extremely Low Turn-on Field. Peter X. Feng, Hongxian Zhang.

**11:40-12:00** **06.14.07**

A Fully Tuneable Microfocus Beamline for Macromolecular Crystallography at Diamond Light Source. Robin Owen, Danny Axford, Jun Aishima, Gwyndaf Evans.

## **06.16 Tips & Tricks of the (Computing) Trade**

**X. Wang, Presiding**  
**Grand Ballroom East**

**09:00-09:30** **06.16.01**

Determination of Problem Structures using SHELX. George Sheldrick

## **06.15 Energy Related Materials**

**A. Huq, Presiding**  
**Grand Ballroom Alley**

**09:00-09:30** **06.15.01**

Structure of  $\text{LiSc}(\text{BH}_4)_4$ : A Novel Salt of  $\text{Li}^+$  and Discrete  $\text{Sc}(\text{BH}_4)_4^-$  Complex Anions. Craig Jensen, Hans Hagemann, Moise Longhini, Radovan Cerny, Magnus Sorby, Bjorn Hauback, Godwin Severa, Jakup Kaminski, Tomasz Wesolowski, Nicolas Penin.

**09:30-09:45** **06.16.02**

Advanced Visualization Tools for Time-of-Flight Laue Single Crystal Neutron Diffraction. Christina Hoffmann, Xiaoping Wang, Dennis Mikkelson, Arthur Schultz, Matthew Frost, Ruth Mikkelson.

**09:30-10:00** **06.15.02**

Materials for Solid Oxide Fuel Cells - Opportunities for Crystallography. Steven McIntosh.

**09:45-10:00** **06.16.03**

Investigation of the Long Range Order and Disorder using JANA2006. Olivier Gourdon, Michal Dusek, Vaclav Petricek, Lukas Palatinus.

**10:00-10:30** Coffee Break.

**10:00-10:30** Coffee Break.

**10:30-11:00** **06.15.03**

The Prediction of Structure and Properties for Rechargeable Li Battery Electrode Materials. Gerbrand Ceder.

**10:30-11:00** **06.16.04**

Quick and Dirty Crystallographic Programming: Past, Present and Future. Joseph Reibenspies.

**11:00-11:30** **06.15.04**

Structural Response to Na Filling in  $\text{Na}_x\text{Si}_{136}$  ( $0 < x < 24$ ) Intermetallic Clathrates Studied by X-ray Powder Diffraction and Rietveld Structure Refinement. Matt Beekman\*, G.S Nolas. \*Powder Diffraction SIG Student Lecturer Awardee

**11:00-11:30** **06.16.05**

What is the Cause of Ghost Peaks Close to Heavy Atoms? Regine Herbst-Irmer, Julian Henn, Daniel Kratzert, Daniel Stern, Dietmar Stalke.

**11:30-12:00** **06.15.05**

Simple and Quick Synthesis of Large-area,

**11:30-12:00** **06.16.06**

What's New in Powder Diffraction Crystallography Software at Argonne's Advanced Photon Source. Brian H. Toby, Robert B. Von Dreele.

# WEDNESDAY, JULY 29

## 01.04 Green Biochemistry

**B. Santariserio, C. Wilmot, Presiding**  
Grand Ballroom West

**01:30-02:15** **01.04.01**

The Joint BioEnergy Institute. Paul Adams, Jay Keasling, Harvey Blanch, Pam Ronald, Blake Simmons.

**02:15-03:00** **01.04.02**

Transport Mechanism of Xenobiotics Across the Bacterial Outer Membrane. Bert van den Berg.

**03:00-03:30** Coffee Break.

**03:30-04:00** **01.04.03**

X-ray Crystallographic Studies of Chlorite Dismutase. Brandon Goblirsch, Bennett Streit, Jennifer DuBois, Carrie Wilmot.

**04:00-04:30** **01.04.04**

Structural Characterization of Catalysis by the Fluoroacetate Dehalogenase from *Rhodospseudomonas palustris* CGA009. Wing Yiu Chan, Alexei Savchenko, Alexander F. Yakunin, Elizabeth A. Edwards, Emil F. Pai.

**04:30-05:00** **01.04.05**

Mechanistic Insight into Methanogenesis Catalyzed by Methyl-coenzyme M Reductase. Peder Cedervall, Mishtu Dey, Xianghui Li, Stephen Ragsdale, Carrie Wilmot.

## 02.02 General Interest

**B. Noll, Presiding**  
Grand Ballroom Centre

**01:30-02:00** **02.02.01**

Ligand's Den: PURY Based Hetero Molecules Geometry Validation Server. Miha Andrejasic, Dusan Turk.

**02:00-02:30** **02.02.02**

Local Area Structural Alignment with ProMOL. Paul Craig, Brett Hanson, Charles Westin, Corey Wischmeyer, Herbert Bernstein.

**02:30-03:00** **02.02.03**

JMOL — A Set of Open-Source Java Ap-

plets for Molecular and Crystallographic Visualization. Patrick Carroll.

**03:00-03:30** Coffee Break.

**03:30-03:45** **02.02.04**

Bubbles, Foam, and the Clathrate Connection. Bryan Chakoumakos.

**03:45-04:00** **02.02.05**

Bringing the Power of Synchrotron Crystallography to the Chemical Community. William Clegg, Ross Harrington, Luca Russo.

**04:00-04:15** **02.02.06**

Improving Data Quality with Multilayer Mirrors. Juergen Graf, Bernd Hasse, Carsten Michaelson.

**04:15-04:30** **02.02.07**

STaRBURSTT-CDC @ YSU: An Update. Matthias Zeller, Allen Hunter.

**04:30-04:45** **02.02.08**

Applicability of Thermofluor and StarGazer-384Tm to Identification of Stabilizing Conditions for Protein-protein Complexes. Jolanta Kopec, Gunter Schneider.

**04:45-05:00** **02.02.09**

The PSI SGKB - A One-stop Shop for Biologists Interested in Protein Structure, Function, Sequence, Methods, and More. John Westbrook, Margaret Gabanyi, Wendy Tao, Raship Shah, Andrei Kouranov, Torsten Schwede, Paul Adams, Lester Carter, Wladek Minor, Helen Berman.

## 03.01 Applications of New Technology in Industry

**M. Peterson, T. Rydel, Presiding**  
Grand Ballroom East

**01:30-02:00** **03.01.01**

Absolute Sgstructure Without Heavy Atoms: Experimental Tests. R.P. Scaringe, J.D. DiMarco, M.F. Malley, M.A. Gallela, M. Dabros.

**02:00-02:30** **03.01.02**

New Technology for Automated and Unattended Crystallographic Structure Determination. Benchtop Systems and High-Intensity Sources. Bruce C. Noll, Michael Ruf, Garold L. Bryant, Jr., Bruce L. Becker, Charles F. Campana, Joerg Kaercher, Stephen M. Leo, Carsten Michaelsen.

**02:30-03:00** **03.01.03**

Pipeline Pilot: A New Take on X-ray Crystallography Refinement Workflows. Francisco Hernandez-Guzman, Yi-Shiou Chen.

**03:00-03:30** Coffee Break.

**03:30-04:00** **03.01.04**

The Effects of UV Irradiation on Protein Crystals. Pierre Le Magueres, Angela Criswell, Bret Simpson.

**04:00-04:30** **03.01.05**

A Metabolome-based Library for Fragment Based Drug Discovery. Douglas Davies, Brian Pease, Bjorn Mamat, Olafur Magnusson, Jeffrey Christensen, Alex Kiselyov, Jasbir Singh, Rama Mishra, Alex Burgin, Lance Stewart.

**04:30-05:00** **03.01.06**

New Monochromator Technology for Improved Data Quality and High Throughput. Roger Durst, Arjen Storm, Charles Campana, Bart Kerpershoek, Bruce Noll, Michael Ruf.

## **04.01 Characterization of Nanomaterials**

**J. Browning, T. Koga, B. Lee, Presiding  
Grand Ballroom Alley**

**01:30-02:00** **04.01.01**

Microphase-separated Structure in a Cylinder-forming Block Copolymer Thin Film Studied by Neutron Reflectivity Aided by Transmission Electron Microtomography. Hiroshi Jinnai, Ken-ichi Niihara, Ukyo Matsuwaki, Naoya Torikai, Hironori Atarashi, Keiji Tanaka.

**02:00-02:30** **04.01.02**

Structure of Membrane-peptide Complexes: From Antimicrobials to Cell Penetrating Peptides. Gerard Wong.

**02:30-02:45** **04.01.03**

Compositional Dependence of the Structure of  $\text{TiO}_2$ :Fe Nanorods. Aleksandar Kremencovic, Bratislav Antic, Emil Božin, Jovan Blanus, Mira Comor, Philippe Colombar, Leo Mazzerolles.

**02:45-03:00** **04.01.04**

Swollen Structures of  $\text{CO}_2$ -philic Polymer Brushes in Density Fluctuating Supercritical Carbon Dioxide. Peter Gin, Mitsunori Asada, Levent Sendogdular, Maya K. Endoh, Hiroki Yamaguchi, Motoyasu Kobayashi, Atsushi Takahara, Tadanori Koga.

**03:00-03:30** Coffee Break.

**03:30-04:00** **04.01.05**

Nanoscope Assemblies of BCP-Based Supramolecules and Nanocomposites in Thin Films. Ting Xu.

**04:00-04:25** **04.01.06**

Layer-by-layer Films Probed by Neutron Reflectivity. Eugenia Kharlampieva, John Ankner, Vladimir Tsukruk.

**04:25-04:50** **04.01.07**

Real Time Snapshot Dynamics of Growing of  $\text{VO}_2$  Nanowires from Supercooled Liquid Nanodroplets. Myung Hwa Kim, Byeongdu Lee, Sungsik Lee, Christopher Larson, Jeong min Baik, Stefan Vajda, Randall E. Winans, Martin Moskovits, Galen D. Stucky, Alec. M. Wodtke.

**04:50-05:05** **04.01.08**

Thin Film Characterization by X-ray Diffraction: In-plane Stress and Strain Components of Epitaxially Grown  $\text{Zn:LiNbO}_3$  Thin Films. Juergen Kraeusslich, Carsten Dubs, Ulf Zastra, Holger Hartung, Andreas Tuennermann.

Registration Desk.....	07:30am .....	Grand Ballroom Foyer
Speaker Ready Room.....	07:30am .....	Conference C
Council Meeting Room.....	07:30am .....	Conference H

## SP.05 Buerger Award

E. Pai, Presiding

Grand Ballroom West

**08:00-08:10** Presentation of Buerger Award to Michael James. Bob Von Dreele, ACA President, Presiding.

**08:10-08:55** **SP.05.01**  
From Sillimanite to Structural Biology or Minerals to Macromolecules. Michael James.

## 01.05 Chromatin Remodeling

J.F. Couture, J. Min, Presiding

Grand Ballroom Centre

**09:00-09:30** **01.05.01**  
Structure, Chemistry and Evolution of Histone Acetyltransferases. Ronen Marmorstein.

**09:30-10:00** **01.05.02**  
Structure and Function of a Yeast Biosynthetic Enzyme Implicated in Chromatin Remodeling. Raymond Trievel, Stacie Bulfer, Erin Scott, Jean-Francois Couture, Lorraine Pillus.

**10:00-10:30** Coffee Break.

**10:30-11:00** **01.05.03**  
Regulation of Histone Deacetylase Activity by Protein-Protein Interaction. Rui-Ming Xu.

**11:00-11:30** **01.05.04**  
Structural and Enzymatic Basis of Cross-talk Between Neighboring Domains in Two Jumonji-Containing Protein Demethylases. John Horton, Anup Upadhyay, Hank Qi, Xing Zhang, Yang Shi, Xiaodong Cheng.

**11:30-11:45** **01.05.05**  
Crystal Structures of CIA/ASF1 HistoneH3-H4 and CIA/ASF1 Bromodomain Complexes Involved in Nucleosome Structural Change. Toshiya Senda, Ryo Natsume, Yusuke Akai, Naruhiko Adachi, Yohei Hayashi, Masamitsu Eitoku, Norihiko Sano, Masami Horikoshi.

**11:45-12:00** **01.05.06**  
Crystallographic Analysis of the Tandem Tudor Domains of Fragile X Mental Retardation Protein 2. Melanie A. Adams-Cioaba, Yahong Guo, Jinrong Min.

## 04.03 SAS Modeling & Applications of SAXS to Biological Problems

G. Beaucage, K. Littrell, Presiding  
Grand Ballroom Alley

**09:00-09:30** **04.03.01**  
Quantification of the Molecular Topology for Hierarchical Macromolecules. Gregory Beaucage, Ramnath Ramachandran.

**09:30-09:45** **04.03.02**  
CO<sub>2</sub> and Methane Sorption in Coal: *in Situ*-Time-Resolved SAXS Investigations. Peter Laggner, M. Schmuck, P. Herrnegger.

**09:45-10:00** **04.03.03**  
Fast Characterization of Proteins in Solution using the SAXSess mc<sub>2</sub> Laboratory SAXS System. Heiner Santner, Heimo Schnablegger, Otto Glatter.

**10:00-10:30** Coffee Break.

**10:30-11:00** **04.03.04**  
The use of Small Angle X-ray Scattering to Determine Structures of Viral Polyproteins from SARS. L. Wayne Schultz, Zachary J. Miknis, Wendy Franke, Timothy C. Umland.

**11:00-11:15** **04.03.05**  
Dissecting Endosomal Escape of Adeno-associated Viruses using X-ray Crystallography and Solution Small-angle Scattering. Balasubramanian Venkatakrisshnan, Mavis Agbandje-McKenna, Mark Porter, Barry Byrne, Sergei Zolotukhin, Nicholas Muzyczka, Lilin He, Robert McKenna.

**11:15-11:30** **04.03.06**  
Biophysical Characterization of the G3 Domain of Agrin Fused with an IgGFc Domain. Trushar Patel, Markus Meier, Shirley Ang, Arthur Rowe, Jianhua Li, Markus Ruegg, Joerg Stetefeld.

**11:30-11:45** **04.03.07**  
SAXS Studies of Non-denaturing SDS-cosolvent Solutions. John Holyoake, Regis Pomes, Gilbert Prive.

## **06.20 Structural Enzymology**

**E. Pai, F. Vajdos**  
**Grand Ballroom West**

**09:00-09:30** **06.20.01**  
Glutathione Reductase: Probing Catalysis at Atomic Resolution. P. Andrew Karplus, Donald S. Berkholz, H. Richard Faber, Savvas N. Savvides.

**09:30-10:00** **06.20.02**  
Structural Basis for the Catalytic Mechanism of Human Phosphodiesterase 9. Sheng-Liu Li.

**10:00-10:30** Coffee Break.

**10:30-11:00** **06.20.03**  
Engineering a Protease into an Allosteric Switch by Stabilization of the Inactive E\* Form. Alaji Bah, Christopher J. Carrell, Zhiwei Chen, Prafull S. Gandhi, Enrico Di Cera.

**11:00-11:20** **06.20.04**  
Structural Characterization of Oxygen Pathways in Cytochrome *ba*<sub>3</sub> Oxidase. Mitch Luna, Ying Chen, James Fee, C. David Stout.

**11:20-11:40** **06.20.05**  
Structural Studies of Truncated Human ATP-Citrate Lyase. Tianjun Sun, Koto Hayakawa, Marie Fraser.

**11:40-12:00** **06.20.06**  
Structures and Substrate Transfer Mechanisms of Eukaryotic Fatty Acid Synthases. Timm Maier, Marc Leibundgut, Simon Jenni, Nenad Ban.

*session continues after lunch at 01:30*

## **06.21 Educational Outreach in Crystallography**

**C. Lind, J. Ng, Presiding**  
**Grand Ballroom East**

### **Revised schedule for 06.21**

**09:00-09:30** **06.21.01**  
Looking at Structures with Diverse Audiences. Christine Zardecki, Shuchismita Dutta.

**09:30-09:45** **06.21.02**  
The Development of www.P212121.com. Sean Seaver.

**09:45-10:00** **06.21.03**  
Bringing the Cambridge Structural Database to Undergraduate Teaching. Gary Battle, Greg Ferrence.

**10:00-10:30** Coffee Break.

**10:30-10:45** **06.21.04**  
The 32 Letter Genetic Code of Anaeromyxobacter dehalogenans. Jimmitti Teysir, William L. Duax, Robert Huether, David Dziak, Dana Hogan, Patrick Ryan.

**10:45-11:00** **06.21.05**  
A Substrate Specific Subset of the Short-Chain Oxidoreductase (SCOR) Superfamily. Tyler Kirsch, Jimmitti Teysir, Dana Hogan, Robert Huether, Sanjay Connare, William L. Duax.

**11:00-11:15** **06.21.06**  
GARP Content Statistics in the PDB Distinguish Bona Fide Proteins from Nonsense Sequences in 169 Microbial Genomes. Ryan Patrick, Jimmitti Teysir, Dana Hogan, Rasheen Powell, Fiona Hennig, Charlotte Lane, Robert Huether, David Dziak, Charles Weeks, William L. Duax.

**11:15-11:45** **06.21.07**  
Five Years, 500 Figures, and 1200 Pages Later: Tales From The Crypt. Bernhard Rupp.

**11:45-12:00** **06.21.08**  
Fourier Transforming My Crystallographic Knowledge At The ACA Summer School. Lorraine Malaspina

**11:15-11:45** **06.21.07**  
Five Years, 500 Figures, and 1200 Pages Later: Tales From the Crypt. Bernhard Rupp.

**11:45-12:00** **06.21.08**  
Fourier Transforming my Crystallographic Knowledge at the ACA Summer School. Lorraine Malaspina.

## **01.06 Carbohydrate Recognition**

**S. Evans, K. Ng, Presiding**  
**Grand Ballroom Centre**

**01:30-01:55** **01.06.01**  
Soluble Lectins from Opportunistic Bacteria Interacting with Host Glycoconjugates. Anne Imberty.

**01:55-02:20** **01.06.02**  
The Crystal Structure of a Sodium Galactose Transporter Reveals Mechanistic Insights into Na<sup>+</sup>/Sugar Symport. Jeff Abramson, Salem Faham, Akira Watanabe, Gabriel Mercado Besserer, Duilio Cascio, Alexander Specht, Bruce Hirayama, Ernest Wright.

**02:20-02:40** **01.06.03**  
Structural Investigations into the Substrate Specificities of Human Maltase-Glucoamylase and Sucrase-Isomaltase in Terminal Starch Digestion. Lyann Sim, David Rose.

**02:40-03:00** **01.06.04**  
Structural Basis of Glycosylation and Reversibility of Glycosyltransferase. Xiaoqiang Wang, Luzia Modolo, Richard A. Dixon.

**03:00-03:30** Coffee Break.

**03:30-03:55** **01.06.05**  
Golgi  $\alpha$ -mannosidase II: Structure, Mechanism and Inhibitor Design. David Rose, Douglas Kuntz, Niket Shah.

**03:55-04:15** **01.06.06**

Crystal Structure and Biochemical Characterization of *Mycobacterium tuberculosis* Ribokinase (Rv2436). Eugene Masters, Yanjie Sun, Yimin Wang, William Parker, Rongbao Li.

**04:15-04:35** **01.06.07**  
ADP-dependent 6-phosphofructokinase from *Pyrococcus horikoshii* OT3: Structure Determination and Biochemical Characterization of PH1645. Mark Currie, Felipe Merino, Tatiana Skarina, Andrew Wong, Alexander Singer, Greg Brown, Alexei Savchenko, Andres Caniguir, Victoria Guixè, Alexander Yakunin.

**04:35-04:55** **01.06.08**  
Structure-Function Analysis of the NDP-Sugar Hydrolase PseG: Unveiling Similarities Between Hydrolases and Glycosyltransferases. Ian Schoenhofen, Erumbi Rangarajan, Ariane Proteau, Qizhi Cui, Susan Logan, Dennis Whitfield, Enrico Purissima, Mirosław Cygler, Allan Matte, Traian Sulea.

## **04.04 Advances in Small-Angle Scattering**

**K. Littrell, F. Zhang, Presiding**  
**Grand Ballroom Alley**

**01:30-02:00** **04.04.01**  
Study of Nanoporous Materials using Coherent X-ray Diffraction Imaging with Crystal Guard Aperture. Qun Shen, Xianghui Xiao, Yong Chu, Hanfei Yan.

**02:00-02:30** **04.04.02**  
Resonance-enhanced Grazing-Incidence Small-Angle X-ray Scattering of Buried Structures in Thin Films. Zhang Jiang, Michael Sprung, Xuefa Li, Suresh Narayanan, Jin Wang.

**02:30-02:45** **04.04.03**  
SAXS-Fiber Computer Tomography. Nanostructure Analysis with Micrometer Spatial Resolution in Fibers and Strands. Norbert Stribeck, Ulrich Nochel.

**02:45-03:00** **04.04.04**

A Novel Approach to the Anomalous Small Angle Scattering (ASAXS) on Au/TiO<sub>2</sub> Catalyst. Sachit Chopra, Gregory Beaucage.

**03:00-03:30** Coffee Break.

**03:30-04:00** **04.04.05**

Polarized SANS Investigation of Magnetic Correlations within Magnetite Nanoparticle Assembly. Kathryn Krycka, Charles Hogg, Yumi Ijiri, Ryan Booth, Julie Borchers, Wangchun Chen, Shannon Watson, Catherine Conlon, James Rhyne, Sara Majetich.

**04:00-04:30** **04.04.06**

Development of Spin-Echo Scattering Angle Measurement (SESAME) for Real-Space Correlation Measurements. Paul Stonaha, Rana Ashkar, Michael Fitzsimmons, Ronald Jones, Wai-Tung Lee, Brian Maranville, Shah Valloppilly, Adam Washington, Roger Pynn.

**04:30-04:45** **04.04.07**

The Center for Structural Molecular Biology (CSMB) at Oak Ridge National Laboratory (ORNL). Volker Urban, William Heller, Kevin Weiss, Hugh O'Neill, Dean Myles.

**04:45-05:00** **04.04.08**

Development of Polarization Analysis in SANS using a Compact Polarized <sup>3</sup>He Neutron Spin Filter. Wangchun Chen, T. R. Gentile, S.M. Watson, K.L. Krycka, M. Laver, J.A. Borchers, G.L. Jones.

## **06.18 Ferroic and Multiferroic Materials**

**P. Gehring, Presiding**  
**Grand Ballroom East**

**01:30-02:15** **06.18.01**

Electric Field Control of Magnetism and Ferroelectricity in Single Crystals of Multiferroic BiFeO<sub>3</sub>. Valery Kiryukhin, S. Lee, T.

Choi, S-W. Cheong, W. Ratcliff, R. Erwin.  
**02:15-03:00** **06.18.02**

Columns and Waterfalls in the Lead based Relaxor Ferroelectric Pb(Mg<sub>1/3</sub>Nb<sub>2/3</sub>)O<sub>3</sub>. Chris Stock, Ian Swainson, Peter Gehring, Xu Guangyong, Viehland Dwight, Luo Hasuo.

**03:00-03:30** Coffee Break.

**03:30-03:55** **06.18.03**

Magnetic Field Effect on Charge Order in the New Multiferroic LuFe<sub>2</sub>O<sub>4</sub>. Jinsheng Wen, Guangyong Xu, Genda Gu, Steve Shapiro.

**03:55-04:20** **06.18.04**

Crystal and Magnetic Structure of FeV<sub>2</sub>O<sub>4</sub>. Sungdae Ji, S. -H. Lee, Q. Huang, T. Kat-sufuji.

**04:20-05:05** **06.18.05**

Spiral Spin Structures and Origin of the Magneto-Electric Coupling in YMn<sub>2</sub>O<sub>5</sub>. Seung-Hun Lee.

## **06.20 Structural Enzymology**

**E. Pai, F. Vajdos, Presiding**  
**Grand Ballroom West**

**01:30-02:00** **06.20.07**

Substrate Recognition and Catalysis of Family 1 and 4 Polysaccharide Lyases. Sine Larsen, Michael McDonough, Majbritt Thymark, Malene H. Jensen, Harm Otten, Leila Lo Leggio, Torben Borchert, Lars H. Christensen, Henrik Frisner, Carsten Sonksen.

**02:00-02:20** **06.20.08**

Structural Insights into Error Prone Replication and Stalling Opposite a Template Thymine Base by Human DNA Polymerase. Kevin Kirouac, Hong Ling.

**02:20-02:40** **06.20.09**

MauG-Catalyzed TTQ Cofactor Synthesis in Methylamine Dehydrogenase (MADH): Crystal Structures of Catalytically Relevant MauG-MADH Complexes. Lyndal Hill,

## THURSDAY, JULY 30

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Teresa De la Mora-Rey, Xianghui Li, Victor Davidson, Carrie Wilmot.

**02:40-03:00** **06.20.10**  
An Unusual Halogenase in Curacin A Biosynthesis. Dheeraj Khare, Liangcai Gu, David H. Sherman, Janet L. Smith.

**03:00-03:30** Coffee Break.

**03:30-04:00** **06.20.11**  
Quantum Catalysis Model Based on Proton Mobility Revealed by Subatomic Resolution X-ray and Neutron *h*-Aldose Reductase structures. Alberto Podjarny, Matthew Blakeley, Federico Ruiz, Oscar Ventura, Andre Mitschler, Pavel Afonine, Raul Cachau, Steven Ginell, Andrzej Joachimiak, Dean Myles.

**04:00-04:20** **06.20.12**  
Revised Mechanism of Sugar Interconversion by Enzyme Xylose Isomerase Employing Time-of-Flight Neutron Crystallography. Andrey Kovalevsky, Zoe Fisher, Marat Mustyakimov, Leif Hanson, Jenny Glusker, Paul Langan.

**04:20-04:40** **06.20.13**  
A Symmetrical Tetramer for *S. aureus* Pyruvate Carboxylase in Complex with Coenzyme A. Linda Yu, Song Xiang, Gorka Lasso, David Gil, Mikel Valle, Liang Tong.

**04:40-05:00** **06.20.14**  
Distortion in Substrate-Product Transition in Orotidine 5'-Monophosphate Decarboxylase. Masahiro Fujihashi, Lianhu Wei, Lakshmi P. Kotra, Emil F. Pai.

## FRIDAY, JULY 31

### 2010 Chicago Meeting Planning Session

**08:30am** Conference B/C

## GENERAL CHEMISTRY



Linus Pauling

## Pauling

The Pauling Poster Prize was established by the ACA, and is supported by member contributions, to honor Linus Pauling. Linus Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each annual meeting the five best student (graduate or undergraduate) poster presentations receive selected as the Trust Fund sponsor.

Winners will be notified before the banquet on Wednesday, July 29.



Canadian National Committee for Crystallography (CNCC)

Pauling awards. In addition, one poster is IUCr winner. The Larry Calvert CNC/IUCr sponsors a prize from a poster from Canadian fore the banquet on Wednesday, July 29.

## Oxford Cryosystems, Inc.

The Oxford Cryosystems Low Temperature Poster Prize is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc. The winner will be announced at the banquet on Wednesday, July 29.



## RCSB Protein Data Bank

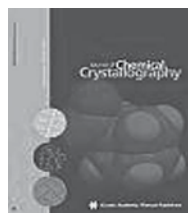
The RCSB PDB Poster Prize

recognizes a student poster presentation involving macromolecular crystallography. The award will be two educational books that will be mailed to the winner after the meeting. An announcement will appear on the PDB Web site and in the PDB Newsletter, and in the ACA and IUCr Newsletters.



## The Journal of Chemical Crystallography

The Journal of Chemical Crystallography proudly sponsors a prize to be awarded to the best student poster presentation in the area of chemical crystallography or small molecule structure determination and analysis at the ACA's Annual Meeting. The winner will receive a one-year subscription to the Journal of Chemical Crystallography and a \$200 Springer book voucher. The winner will be announced at the banquet on Wednesday, July 29.



# Posters

Posters beginning with **P-S** should be assembled before 05:00pm on Sunday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with **P-M** should be assembled before 05:00pm on Monday and be removed at the conclusion of the poster session at 7:30pm.

Posters beginning with **P-T** should be assembled before 05:00pm on Tuesday and be removed at the conclusion of the poster session at 7:30pm.

**Please be present at your poster during the entire time on the day to which you are assigned.**

## Sunday Posters

### P-S001

From PyMOL Session Files to Jmol State Scripts: The Proteopedia PyMOL2Jmol Translator. Roni Gordon, Eran Hodis, Jaime Prilusky, Joel Sussman.

### P-S002

Structural Analysis of DEAD Box 1 (DDX1) Protein. Matthew Hildebrandt, Bart Hazes, Roseline Godbout.

### P-S003

Structure of Monomeric Isocitrate Dehydrogenase Holoenzyme from *Corynebacterium glutamicum*. Navdeep Sidhu, Louis TJ Delbaere.

### P-S004

Time-resolved Laue Diffraction of the Reaction Center of *Blastochloris viridis*. Linda Johansson, Erik Malmerberg, Gergely Katona, Annemarie Wöhri, Richard Neutze.

### P-S005

The Crystal Structure of TraM bound to *oriT* DNA from the F-type Plasmid pED208. Joyce Wong, Jun Lu, Ross A. Edwards, Laura S. Frost, J. N. Mark Glover.

### P-S006

Structural Studies of GfcC, a Protein Essential for Capsule Polysaccharide Expression by Pathogenic *E. coli*. Karthik Sathiyamoorthy, Mark Saper.

### P-S007

Structural and Functional Characterization of a Novel Cupin Protein from the Pathogenic *E. coli* O157:H7. Laura van Staaldunen, Zongchao Jia.

### P-S008

Crystal Structure of the MIF4G of the Poly(A)-binding Protein-interacting Protein 1 (PAIP1). Ahmad Kanaan, Fillipp Frank, Nahum Sonenberg, Bhushan Nagar.

### P-S009

Investigation into the Cause of Disparate Macromolecular Space Group Frequencies. Colin McCrimmon, Cameron Mura.

### P-S010

Crystal Structure of *Streptococcus agalactiae* Pilus-specific Sortase, Sortase B. Baldeep Khare, Kevin Macon, Dwight Moore, Hung Ton-That, Sthanam V. L. Narayana.

### P-S011

On the Detection, Analysis and Prediction of Allosteric Information Pathways Derived from Human Serum Albumin Crystallographic Data. Horacio Botti, Felipe Trajtenberg, Bruno Manta, Otto Pritsch, Alejandro Bushiazzo.

### P-S012

Microdiffraction: What Can be Done? Kanagalaghatta Rajashankar (Raj), Malcolm Capel, Stephen Harrison, Steve Ealick.

### P-S014

The 3.6 Å Structure of the RNA Surveil-

lance Protein Mtr4 Reveals a Novel Arch Domain. Ryan Jackson, Bradley Hintze, Sean Johnson.

**P-S015**

Iron Storage by Ferritin in Bloom-forming Marine Pennate Diatoms. Stephanie Pfaffen, Angele Arrieta, Lauren Moccia, Maria Maldonado, Michael Murphy.

**P-S016**

Towards the Structure of ER  $\alpha$  Glucosidase I. Megan K. Barker, David R. Rose.

**P-S017**

X-ray Crystal Structure of *Yersinia pestis* Plasminogen Activator Pla. Elif Eren, Jon Goguen, Bert van den Berg.

**P-S018**

Structural Studies on  $\alpha$ -Kinase Domain of Dictyostelium Myosin II Heavy Chain. Qilu Ye, Scott W. Crawley, Yidai Yang, Cote P. Graham, Zongchao Jia.

**P-S019**

A Pentameric Coiled Coil as a Carrier-Pathfinder System for 5-Fluorouracil. Ainsley McFarlane, Nasrin Mesaeli, George Orriss, Jorg Stetefeld.

**P-S020**

Structural Basis for Specific Recognition of Multiple mRNA Targets by a PUF Regulatory Protein. Yeming Wang, Laura Opperman, Marvin Wickens, Traci Hall.

**P-S021**

Structural Analysis of C-terminal of Hsc70 Interacting Protein (CHIP) Mediated Protein Quality Control Network. Zhen Xu, Richard C. Page, Saurav Misra.

**P-S022**

Crystal Structure of UDP-galactopyranose Mutase in Complex with Substrate and Inhibitor. Sarathy Karunan Partha, David Sanders.

**P-S023**

Crystal Structure of the DAP5/p97 mIF4G-Domain. Philipp Frank, Genevieve Virgili, Nahum Sonenberg, Bhushan Nagar.

**P-S024**

Structural Biology of Rift Valley Fever Virus Nucleoprotein. Donald Raymond, Mary Piper, Sonja Gerrard, Janet Smith.

**P-S025**

Characterizing a Novel Hemophore from Pathogenic and Non-pathogenic Mycobacteria. Lisa Marie McMath, Michael Tullius, Lana Cong, Nicholas Chim, Christine Harmston, Sylvia Soo, Marcus Horwitz, Celia Goulding.

**P-S026**

Preparation of the Ebola Virus Glycoprotein for Structural Characterization Related to Development of a Multiepitope Vaccine. Dayong Zhou, Hao Xu, Frank Michel, Jeff Hogan, John Rose.

**P-S027**

The Phox Domain of Sorting Nexin 5 Lacks Ptdins(3)P Specificity and Preferentially Binds to Ptdins(4,5)P2. Mohamad Koharudin, William Furey, Hao Liu, Yong-Jian Liu, Angela Gronenborn.

**P-S028**

Molecular Mechanism of the Distinct Salt-dependent Enzyme Activity of two Halophilic Nucleoside Diphosphate Kinases. Akihiro Yamamura, Takefumi Ichimura, Masahiro Kamekura, Toru Mizuki, Ron Usami, Tsukasa Makino, Jun Ohtsuka, Ken-ichi Miyazono, Koji Nagata, Masaru Tanokura.

**P-S029**

Yeast Aquaporin Gating - A Membrane Protein at 1.15 $\approx$  Resolution. Gerhard Fischer, Urszula Kosinska-Eriksson, Madelene Palmgren, Camilo Aponte-Santamaria, Kristina Hedfalk, Bert deGroot, Stefan Hohmann, Richard Neutze, Karin Lindkvist-Pettersson.

## Posters-S

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### P-S030

Crystal structure of REV7. Kodai Hara, Toshiyuki Shimizu, Yoshiki Murakumo, Tomo Hanafusa, Haruo Ohmori, Mamoru Sato, Hiroshi Hashimoto.

### P-S031

Structural Study for Regulation Mechanism of Plant NADPH Oxidase. Takashi Oda, Hiroshi Hashimoto, Naoyuki Kuwabara, Kokoro Hayashi, Chojiro Kojima, Hann Ling Wong, Tsutomu Kawasaki, Ko Shimamoto, Mamoru Sato, Toshiyuki Shimizu.

### P-S032

Structural and Functional Characterization of Human P2 Protein from Peripheral Nervous System Myelin. Viivi Majava, Rahul Nanekar, Petri Kursula.

### P-S033

Architecture of Human NHEJ Ligation Complex. Meghan McFadden, Pei-Yu Wu, Philippe Frit, SriLakshmi Meesala, Stephanie Dauvillier, Mauro Modesti, Sara. N. Andres, Ying Huang, JoAnn Sekiguchi, Murray S. Junop.

### P-S034

The Structure of Rabbit PrPC: Structural Clues into the Species Barrier and Prion Disease Susceptibility. Braden Sweeting, Avi Chakrabarty, Emil F. Pai.

### P-S035

Structures of the Essential RNA Splicing Factor, U2AF65 Bound to Alternative Polypyrimidine Tracts. Jermaine Jenkins, Katie Frato, Clara Kielkopf.

### P-S036

Crystal Structure of Iodotyrosine Deiodinase, a Novel Flavoprotein Responsible for Iodide Salvage in Thyroid Glands. Seth Thomas, Patrick McTamney, Jennifer Adler, Nicole LaRonde-LeBlanc, Steven Rokita.

### P-S037

Structural Basis for Cell Adhesion Mol-

ecule Recognition by an Armadillo Protein. Noboru Ishiyama, Shuang Liu, Guang-Yao Li, Mitsuhiro Ikura.

### P-S038

Crystal Structure of GAF Domain of Phosphodiesterase-5 and Implications on cGMP Signaling. Huanchen Wang, Howard Robinson, Hengming Ke.

### P-S039

Crystallization and Preliminary X-ray Diffraction of a Hyperactive Ca<sup>2+</sup>-dependent Antifreeze Protein from the Antarctic bacterium *Marinomonas primoryensis*. Christopher P. Garnham, Robert L. Campbell, Peter L. Davies.

### P-S040

Domain Organization of *Clostridium botulinum* Neurotoxin Type E Reveals its Faster Translocation. Desigan Kumaran, Subramaniam Eswaramoorthy, William Furey, Jorge Navaza, Sax Martin, Subramanyam Swaminathan.

### P-S041

Structural Studies of Ebolavirus VP35. Christopher Kimberlin, Erica Ollmann Saphire.

### P-S042

Structural Analysis of the Human Ubiquitin-activating Enzyme 5 (Uba5). John-Paul Bacik, John Walker, Nasrin Rastgoo, Johan Weigelt, Chas Bountra, Cheryl Arrowsmith, Aled Edwards, Alexey Bochkarev, Sirano Dhe-Paganon.

### P-S043

Crystallographic Studies of the Cytoplasmic Domain of the Histidine Kinase DesK from *Bacillus subtilis*. Felipe Trajtenberg, Daniela Albanesi, Mariana Martin, Cecilia Mansilla, Pedro Alzari, Diego de Mendoza, Alejandro Buschiazso.

### P-S044

The Structural Basis of DNA Binding and

Oligomerization by the *E. coli* Antitoxin MqsA (b3021/YgiT). Breann L. Brown, Simina Grigoriu, Jennifer Arruda, Rebecca Page.

**P-S045**

Novel Minimal Substrate Binding by BtuB. Peter Horanyi, Michael Wiener.

**P-S046**

Structural Investigation of a Viral DNA Packaging Molecular Motor. Carina Buttner, Maria Chechik, Miguel Ortiz-Lombardia, Alfred A. Antson.

**P-S047**

Mechanism of EphA2 Receptor Tyrosine Kinase Clustering. Laila Yermekbayeva, John Walker, Martin Lackmann, Dimitar Nikolov, Sirano Paganon.

**P-S048**

Structural Deformations of Bacteriochlorophyll-a as Reveled in a 1.25 $\approx$  Resolution Model of FMO from *Prosthecochloris aestuarii* 2K. Dale Tronrud, Jianzhong Wen, Leslie Gay, Robert Blankenship, P. Andrew Karplus.

**P-S049**

From Bent Crystals to Allosteric Mechanism: The Long-sought and Deeply Asymmetric Structure of the apo CRP Homodimer. Travis Gallagher, Prasad Reddy.

**P-S050**

The Autotransporter Protease EspP: Crystal Structure and Relation to the Human Coagulation Cascade. Shekeb Khan, Hira Mian, Linda Sandercock, Kevin Kuo, Emil Pai.

**P-S051**

Crystal Structure of Human Importin  $\alpha$  (Rch1). Hideyuki Miyatake, Akira Sanjoh, Go Matsuda, Naoshi Dohmae, Yoko Aida.

**P-S052**

Crystal Structure of 2-(5-chloro-3,3-dimethyl-2,3-dihydro-1H-inden-1-yl)piperi-

dinium chloride. Mark Frisch, Jeffrey R. Deschamps, Mark Froimowitz, Charles J. Kelley.

**P-S053**

The Crystalline Characterizations of Single-walled Carbon Nanotubes Grown on Nickel Filled Carbon Nanofibers. Hongxin Zhang, Peter Feng.

**P-S054**

Oligomerization and Structural Analysis of the Type IV Pilins from *Pseudomonas aeruginosa*. Stephanie Lombardo, Gerald F. Audette.

**P-S055**

Variable Temperature Diffraction Studies of A<sup>10</sup>B<sup>14</sup>M<sub>3</sub>O<sub>12</sub> Materials. Tamam Baiz, Cora Lind.

**P-S056**

Charge Density Study of Agostic (C-C) $\rightarrow$ Ti Interactions in Ti(C<sub>5</sub>H<sub>4</sub>Me)<sub>2</sub>(CH<sub>2</sub>)<sub>2</sub>CMe<sub>2</sub>. Stephan Scheins, Mateusz Pitak, Marc Messerschmidt, Milan Gembicky, Gregory C. Turpin, Benjamin G. Harvey, Atta M. Arif, Anatoliy Volkov, Richard D. Ernst, Philip Coppens.

**P-S057**

Analysis of Pore-forming Structures from Northeast Structural Genomics (NESG). Seetharaman Jayaraman, A.P. Kuzin, F. Frouhar, S.M. Vorobiev, M. Su, H. Neely, M. Abashidze, Y. Chen, S. Lew, L. Tong.

**P-S058**

Structure of Q9HYA2, a Short Chain Oxidoreductase from *Pseudomonas aeruginosa* Reveals Novel Catalytic Center Differences. Robert Huether, Vladimir Pletnev, Timothy Umland, William Duax.

**P-S059**

Crystal Structure and Magnetic Properties of the Cobaltite Series (Ba, Sr)<sub>8-x</sub>LaxCo<sub>4</sub>O<sub>15</sub>. Ovidiu Garlea, R. Jin, E. Garlea, R. Custelcean, H. Sha, J. Zhang.

## Posters-S

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### P-S060

Non-Collinear Antiferromagnetism in Fe-CrAs. Ian Swainson, Wenlong Wu, Alix McCollam, Stephen Julian.

### P-S061

Structure and Magnetic Order in Bismuth doped Rare-earth Perovskites. Craig Bridges, Athena Sefat, Lachlan Cranswick, Andrew Payzant, Mariappan Paranthaman.

### P-S062

Spin-state Transition in Lightly Ni Doped LaCoO<sub>3</sub>. Juan Yu, Despina Louca, Daniel Phelan, Yiming Qiu, John Copley.

### P-S063

LABELIT: Extending Automation to Special Cases. Nicholas Sauter, Billy Poon, Peter Zwart, Pavel Afonine, Ralf Grosse-Kunstleve, Paul Adams.

### P-S065

CCP4 6.1 - The Latest Release of the Protein Crystallography Software Suite. Ronan Keegan, Charles Ballard, Norman Stein, Martyn Winn.

### P-S066

Mining the Protein Data Bank to Differentiate Error from Structural Variation in Clustered Static Structures of HIV Protease. Miorel-Lucian Palii, Balasubramanian Venkatakrishnan, Mavis Agbandje-McKenna, Robert McKenna.

### P-S067

Matching PXRD of Crystalline Bulk with the Simulated Pattern of Single-crystal Structure, and Vice Versa. Qi Gao.

### P-S068

Characterization of PilP: A Protein Required for the Assembly of *Pseudomonas aeruginosa* Type 4 Pili. Stephanie Tammam, Priyanka Sundaram, Jason Koo, Melissa Ayers, Andrew Chong, Lili Sampaleanu, Julie Forman-Kay, Lori Burrows, P. Lynne Howell.

### P-S069

*Pseudomonas aeruginosa* PilO Crystal Structure Offers Insight into PilN/O Heterodimerization. Liliana Sampaleanu, Jason Koo, Stephanie Tammam, Melissa Ayers, Jefferey Bonanno, Steven Almo, Stephen Burley, Lori Burrows, Lynne Howell.

### P-S070

Expression, Refolding, Crystallization and Preliminary X-ray Analysis of *Pseudomonas aeruginosa* AlgE. John Whitney, A. Mirela Neculai, Dennis Ohman, P. Lynne Howell.

### P-S071

Crystal Structure of Glycerol-3-Phosphate Dehydrogenase, an Essential Monotopic Membrane Enzyme. Joanne Yeh, Shoucheng Du, Unmesh Chinte.

### P-S072

Functional Activity and Polypeptide Chain Refolding in Allosterically Controlled Type II Citrate Synthases. Gary Brayer, Robert Maurus, Nham Nguyen, Lynda Donald, Harry Duckworth.

### P-S073

Structure Determination of the *Drosophila melanogaster* Peroxisomal Multifunctional Enzyme Type 2 (MFE-2). Tatu Haataja, Kalervo Hiltunen, Tuomo Glumoff.

### P-S074

Characterization of a New Adenylating Enzyme Family Involved in Bacterial Siderophore Biosynthesis. Stefan Schmelz, Nadia Kadi, Stephen McMahon, Kenneth A. Johnson, Lester Carter, Catherine H. Botting, Malcolm F. White, Gregory L. Challis, James H. Naismith.

### P-S075

Crystal Structures of *M. tuberculosis* Ornithine Acetyltransferase and its Complex with Ornithine: A Structural Basis for the Catalytic Mechanism. R. Sankaranarayanan, M.M. Cherney, C. Garen, G. Garen, M. Yuan, M.N.G. James.

**P-S076**

Joint Neutron and X-ray Crystallographic Study of Human Carbonic Anhydrase II (HCA II). S. Zoe Fisher, Andrey Kovalovsky, Marat Mustyakimov, John Domsic, Robert McKenna, Paul Langan.

**P-S078**

Contribution of Zinc to the Stability of Human Carbonic Anhydrase II: Implications of the Loss of the Metal. Balendu Avvaru, Scott Busby, Michael Chalmers, Patrick Griffin, David Silverman, Robert McKenna.

**P-S079**

Characterization of 3-ketosteroid 9 $\alpha$ -hydroxylase, a Rieske Oxygenase in the Cholesterol Degradation Pathway of *Mycobacterium tuberculosis*. Igor D'Angelo, Jenna Capyk, Natalie Strynadka, Lindsay Eltis.

**P-S080**

The Role of an Omega-loop in PEPCCK Mediated Catalysis. Troy Johnson, Todd Holyoak.

**P-S081**

Structural Basis of Substrate Specificity of Haemophilus Influenzae e (P4) Acid Phosphatase. Harkewal Singh, Thomas Reilly, John Tanner.

**P-S082**

The Promiscuous Nature of Althiazide in Adducts with CA II and CA IX Mimic. Jeanne Qurit, Arthur Robbins, James Rocca, Caroli Genis, Mavis Agbandje-McKenna, Robert McKenna.

**P-S083**

Structure of Bifunctional PutA: Evidence for Substrate Channeling. Dhiraj Srivastava, John Tanner.

**P-S084**

Entrapment of Carbon Dioxide in the Active Site of Carbonic Anhydrase II. John Domsic, Balendu Avvaru, Chae Un Kim, Sol Gruner, Mavis Agbandje-McKenna, David Silverman, Robert McKenna.

**P-S085**

Crystal Structure of Diaminopimelate Epimerase from *Arabidopsis thaliana*, an Amino Acid Racemase Critical for L-lysine Biosynthesis. Bindu Pillai, V.A. Moorthie, M.J. van Belkum, S.L. Marcu, M.M. Cherney, C.M. Diaper, J.C. Vederas, M.N.G. James.

**P-S086**

Examination of Substrate Binding Provides Mechanistic Insight into Inositol Phosphate Degradation by Protein Tyrosine Phosphatase Like Phytases. Robert Gruninger, Selina Dobing, Adam D. Smith, Hans-Joachim Wieden, Brent Selinger, Steven C. Mosimann.

**P-S087**

Determination of the Mechanism of 5-Methylthioribose Kinase. K. Dawson, S.Y. Ku, P. Yip, P. L. Howell.

**P-S088**

Structural and Functional Characterization of Yeast Glycogen Synthase. SulochanaDevi Baskaran, Peter J. Roach, Thomas D. Hurley.

**P-S089**

Structural and Biochemical Studies on HpxO, a Novel FAD-Dependent Urate Oxidase from *Klebsiella pneumoniae*. Katherine Hicks, Sean O'Leary, Tadhg Begley, Steven Ealick.

**P-S090**

Understanding the Molecular Basis of Substrate Specificity in 5'-methylthioadenosine/S-adenosylhomocysteine Nucleosidases. K.K.W. Siu, K. Asmus, K.A. Cornell, V.L. Woods, P.L. Howell.

**P-S091**

Binding of 2'-amino-2'-deoxycytidine-5'-triphosphate to Norovirus Polymerase Induces a Conformational Change in the Active Site. Dmitry F. Zamyatkin, Francisco Parra, Angeles Machin, Pawel Grochulski, Kenneth K.-S. Ng.

## Posters-S

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### P-S092

Structural Characterization of the PLP Degradative Enzyme 2-(Acetamidomethylene) succinate Hydrolase. Kathryn McCulloch, Tathagata Mukherjee, Tadhg Begley, Steven Ealick.

### P-S094

Structure and Mechanism of an RNA Polymerase-Associated Swi2/Snf2 Protein: How RapA Completes the Transcription Cycle. Gary Shaw, Yan Ning Zhou, Priadarsini Subburaman, Ding Jun Jin, Xinhua Ji.

### P-S095

Crystal Structure and Catalytic Mechanism of an Enzyme in the Fungal Lysine Biosynthetic Pathway. Stacie Bulfer, Erin Scott, Jean-Francois Couture, Lorraine Pillus, Raymond Trievel.

### P-S096

Structural Studies of Modular Poyketide Synthase Systems: The Dehydratase Domains from the Curacin Pathway. David Akey, Jason Tehranisa, Jamie Razelun, Janet Smith.

### P-S097

Dynamic Role of SecA DEAD Motor in Protein Translocation. Stanley Nithianantham, Brian Shilton.

### P-S098

The Crystal Structure of THI6, a Bifunctional Enzyme Involved in Thiamin Biosynthesis in Eukaryotes. Debamita Paul, Tadhg Begley, Steven Ealick.

### P-S099

Structural Insights into Inorganic NO Donors as Inhibitors of *Trypanosoma cruzi* Glyceraldehyde-3-Phosphate Dehydrogenase. Tatiane Balliano, Rafael Guido, Francisco Silva, Luis Lopes, Jean Silva, Adriano Andricopulo, Glaucius Oliva.

### P-S100

Structural Characterization of LinB, an Adenylyltransferase Responsible for Lincosamide Resistance. Mariya Morar, Gerard Wright, Kirandeep Bhullar.

### P-S101

Crystal Structure of a Key Complex from the Pseudomonas Quinolone Signal Biosynthesis Pathway. Asim K. Bera, Vesna Atanasova, Everett C. Pesci, James P. Coleman, James F. Parsons.

### P-S102

A Sucrose Binding Mutant of MBP Provides Insights into the Mechanism of the *Escherichia coli* Maltose Transporter. Alister Gould, Brian Shilton.

### P-S103

Structural and Kinetic Insight into Severe Substrate MgATP Inhibition of Pyridoxal Kinase in the Presence of its Enzymatic Product. Amit Gandhi, Faik Musayev, Mohini Ghatge, Verne Schirch, Martin Safo.

### P-S104

Structure-Function Effects of Active Site Mutations in the *E. coli* Pyruvate Dehydrogenase Multienzyme Complex E1 Component. Palaniappa Arjunan, Natalia Nemeria, Frank Jordan, William Furey.

### P-S105

Kinetic Associations of DCoH Regulate HNF-1a Activity in Diabetes. Helen Rho, Chasity Jones, Robert Rose.

### P-S106

Structural Investigation of Cofactor Biosynthesis in a Copper Amine Oxidase from *Hansenula polymorpha*. Valerie Klema, Bryan Johnson, Jennifer DuBois, Judith Klinman, Carrie Wilmot.

### P-S107

Structural Studies of *Streptococcus Pyogenes* Uridine Phosphorylase. Timothy

Tran, Jure Piskur, Steven Ealick, S. Christoffersen, I. Serra, M. Terreni.

**P-S108**

Multiple Conformers in Active Site of Human Dihydrofolate Reductase F31R/Q35E Double Mutant Suggest Structural Basis for Methotrexate Resistance. Brahm Jonathan Yachnin, Jordan Volpato, Jonathan Blanchet, Vanessa Guerrero, Lucie Poulin, Elena Fos-sati, Joelle N. Pelletier, Albert M. Berghuis.

**P-S109**

X-ray Crystallographic Studies of the Aminoglycoside Modifying Enzyme APH(2'')-Id. Kun Shi, Albert Berghuis.

**P-S110**

Structural Basis for the Activities of FG41 MSAD. Youzhong Guo, Hector Serrano, William Johnson, Chris Whitman, Marvin Hackert.

**P-S111**

The Crystal Structure of a Novel AroE-like Shikimate Dehydrogenase from *Pseudomonas putida*. James Peek, Sasha Singh, Kay Chen, Dinesh Christendat.

**P-S112**

High-resolution Structure of Acetate Kinase from *Cryptococcus neoformans*. Tarjani Thaker, Cheryl Ingram-Smith, Ashley Lawhon, Kerry Smith, Tina Iverson.

**P-S113**

Evidence of a Copper-dependent Iron Transport Role for the *Campylobacter jejuni* Protein P19. Anson Chan, Tzanko Doukov, Melanie Scofield, Stacey Tom-Yew, Alexander Ramin, Erin Gaynor, Michael Murphy.

**P-S114**

The Crystal Structure of *A. aeolicus* Prephenate Dehydrogenase Reveals the Mode of Tyrosine Inhibition. Dinesh Christendat, Warren Sun, Dea Shahinas, Julie Bonvin, Wenjuan Hou, Joanne Turnbull.

**P-S115**

Crystal Structure Determination of Feline Calicivirus Proteinase-Polymerase. Isabelle Barrette-Ng, Angela Fan, Craig E. Cameron, Kim Y. Green, Stanislav V. Sosnovtsev, Kenneth K. S. Ng.

**P-S116**

Crystal Structures of Human Senescence Marker Protein-30 (SMP30): Identification and Characterization of the Gluconolactonase Active-site. Subhendu Chakraborti, Brian Bahnson.

**P-S117**

The Acid Stress Response in Bacteria: The Role of the Novel AAA+ ATPase RavA. Majida El Bakkouri, Miao Yu, Usheer Kanjee, Wim Pascal Burmeister, Guy Schoehn, Irina Gutsche, Walid A. Houry.

**P-S118**

Studies of Enzymes Involved in Modification of tRNA Wobble Position. Rong Shi, Ariane Proteau, Magda Villarroya, I. Moukadiri, Linhua Zhang, Eugenia Armengod, Allan Matte, Mirosław Cygler.

**P-S119**

GARP Content of Ribosomal Proteins Reveals their Origin in GC-Rich Species. Rasheen Powell, Fiona Hennig, Robert Huether, David Dziak, Charles Weeks, William L. Duax.

**P-S120**

Codon use in GC-Rich Species Reveals the Order of Evolution of Codon Definitions. Fiona Hennig, Charlotte Lane, Patrick Ryan, Rasheen Powell, Emma Rutkowski, Kevin Gibas, Robert Huether, David Dziak, Charles Weeks, William L. Duax.

## Monday Posters

### P-M001

Structural Insight into *Homoserine Transacetylase* from *Haemophilus influenzae*. Magdalena Korczynska, I. Ahmad Mirza, Albert M. Berghuis.

### P-M002

Crystal Structure of CmlS: A Flavin-dependent Halogenase from Chloramphenicol Biosynthesis Pathway of *Streptomyces venezuelae*. Kateryna Podzelinska, Ryan Latimer, Alexei Soares, Anupam Bhattacharya, Leo Vining, David Zechel, Zongchao Jia.

### P-M003

Crystal Structure of the *Bacillus subtilis* Bacteriophage  $\tau$ 29 Prohead RNA. Ailong Ke, Ding Fang, Anderson Dwight, Lu Changrui, Grimes Shelley.

### P-M004

Examining the Structural Basis of Ubiquitin Ligase Self-Assembly and its Implication as a Regulatory Switch. Wesley Errington, Ashley Ross, Peter Stogios, Gilbert Prive.

### P-M005

The Structural Basis of Heme Transfer in the Cell Surface Isd System from *Staphylococcus aureus*. Jason Grigg, Cherry Mao, Michael Murphy.

### P-M006

Structural and Biochemical Insights into the MST-FOXO Signaling Pathway. Ruchi Anand.

### P-M007

Structural Basis of Transcription Activation by the Cyclin T1-Tat-TAR RNA Complex. Kanchan Anand, Antje Schulte, Karin Vogel Bachmayr, Klaus Scheffzek, Matthias Geyer.

### P-M008

The 1.6  $\approx$  Structure of the *Helicobacter pylori* Urease Accessory Protein UreF. Robert

Lam, Vladimir Romanov, Robert Hausinger, Kathy Johns, Kevin Battaile, Jean Wu-Brown, Emil Pai, Nickolay Chirgadze.

### P-M009

Structural and Enzymatic Characterization of Mitochondrial HAD-like Phosphatase from *Saccharomyces cerevisiae*. Bogi Nock, Kate Kuznetsova, Elena Evdokimova, Alex Savchenko, Aled Edwards, Alexander Yakunin, Andrzej Joachimiak.

### P-M010

Structural and Functional Insights into Roles of the Mms21 Subunit of the Smc5/6 Complex. Xinyuan Duan, Hong Ye.

### P-M011

The Crystal Structure of the *Mycobacterium tuberculosis* Rv3019c-Rv3020c ESX Complex Reveals a Domain-swapped Heterotetramer with Functional Implications. Mark Arbing, Markus Kaufmann, Tung Phan, Sum Chan, Dulio Cascio, David Eisenberg.

### P-M012

CAP-dependent Transcription Initiation Subassembly Based on Multiple Crystal Structures. Samuel Lara-Gonzalez, Jens Birktoft, Richard Ebright, Helen Berman, Catherine Lawson.

### P-M013

Structural Details of HIV-1 Recognition by the Broadly Neutralizing Monoclonal Antibody 2F5: Epitope Conformation, 2F5 CDR H3 Loop Mobility and Anion-binding Site. Jean-Philippe Julien, Steve Bryson, Jose L. Nieva, Emil F. Pai.

### P-M014

Structural Studies of the Hepatitis B Virus Surface Protein (HBsAg) Aimed at Developing Next Generation Vaccines. Quentin Florence, Hao Xu, Jonny Yokosawa, James Lara, Yuri Khudiyakov, John P. Rose.

### P-M015

Crystal Structures Reveal a Shared Immu-

nological Solution for Neutralizing Ebolaviruses. Joao Dias, Ana Kuehne, John M. Dye, Erica Ollmann Saphire.

**P-M016**

Structural Insights into Immune Recognition of the Severe Acute Respiratory Syndrome Coronavirus S Protein Receptor Binding Domain. John E. Pak, Chetna Sharon, Thierry C. Auperin, Cheryl M. Cameron, David J. Kelvin, Jayaraman Seetharaman, Alan Cochrane, Francis A. Plummer, Jody D. Berry, James M. Rini.

**P-M017**

Immune Evasion at the Site of CD4 Binding on HIV-1 gp120. Lei Chen, Young Do Kwon, Tongqing Zhou, Xueling Wu, Sijy O Dell, Ann J. Hessel, Min Tang, Ling Xu, Zhi-yong Yang, Peter D. Kwong.

**P-M018**

Structural Studies on Hepatitis E Virus Capsid Protein. J Sivaraman, Shaowei Li, Xuhua Tang, Chunyan Yang, Choy Leong Hew, Ningshao Xia.

**P-M019**

Polymer-Induced Heteronucleation as an Enabling Technology in Protein Crystallization. Leila Foroughi, A.J. Matzger.

**P-M020**

The Microcapillary Protein Crystallization System (MPCS). Cory Gerdt, Peter Nollert, Mark Elliot, Qiang Fu, Liang Li, Rustem Ismagilov, Lance Stewart.

**P-M021**

Protein Crystallization: Robotics, Procedures and Developments. Fabrice Gorrec, Olga Perisic, Katharine Michie, Gebhard Schertler, Jan Lowe.

**P-M022**

Manipulating Tool for Protein Microcrystals in Solution using Adhesive Materials. Kazufumi Takano, Tomoya Kitatani, Hiroaki Adachi, Shigeru Sugiyama, Hiroyoshi

Matsumura, Ryota Murai, Yoshinori Takahashi, Satoshi Murakami, Tsuyoshi Inoue, Yusuke Mori.

**P-M023**

Polystyrene Nanospheres in Crystallization of Proteins. Nina Hakulinen, Johanna Kallio, Juha Kallio, Merja Niemi, Susanna Kärkkäinen, Juha Rouvinen.

**P-M024**

Crystal Structure of an Adenylosuccinate Lyase from *Legionella pneumophila*. Hui Li, Cs. Chang, L. Freeman, F. Collart, A. Joachimiak.

**P-M025**

Effect of Leucine-to-methionine Substitutions on the Diffraction Quality of Histone Chaperone SET/TAF-I $\beta$ /INHAT Crystals. Miki Senda, Shinsuke Muto, Masami Horikoshi, Toshiya Senda.

**P-M026**

Protein Crystallization using the Crystal Former Microfluidic Device. Morten O. A. Sommer, Vivian Stojanoff, Jean Jakoncic.

**P-M027**

X-Ray Transparent Crystallization Plates for High Performance Protein Crystallization. Ahmed Soliman, Benjamin Apker, Yevgeniy Kalinin, Robert Thorne.

**P-M028**

Structural Analyses of the Alleged Manno-6-phosphate Transferase from *Saccharomyces cerevisiae*. Daniella Marks, Dmitry Rodionov, Pedro A. Romero, Annette Herscovics, Albert M. Berghuis.

**P-M029**

Lysozyme Crystallization on Siloxane Monolayers. Lindsey E. Roeker, Ilana G. Goldberg, Jennifer A. Swift.

**P-M030**

Towards the Atomic Structure of Tenascin C Assembly Domain. Markus Meier, Trushar Patel, S.Ozbek, Jorg Stetefeld.

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### P-M031

Techniques and Tactics used in Determining the Structure of the Trimeric, Prefusion Ebola Virus Glycoprotein. Jeffrey Lee, Marnie L. Fusco, Erica Ollmann Saphire.

### P-M032

Diffraction-Capable Microfluidic Crystallization Chips for Screening and Structure Determination. Andrew May, Brian Fowler, Ken Frankel, George Meigs, Scott Gradia, Chris Jeans, James Berger, James Holton.

### P-M033

To G or not to G. Bart Hazes.

### P-M034

Crystallization Image Analysis on the World Community Grid. Christian Cumbaa, Igor Jurisica.

### P-M035

Towards the Development of X-ray Transparent Devices for *in situ* Crystal Growth and X-ray Diffraction Data Collection. Matthew Engel, Alexei Soares, Allen Orville, Marc Allaire.

### P-M036

Improvement of Femtosecond Laser-induced Nucleation Efficiency in a Highly Viscous Solution. Ryota Murai, Hiroshi Yoshikawa, Natsuko Iefuji, Yoshinori Takahashi, Hiroaki Adachi, Kazufumi Takano, Hiroyoshi Matsumura, Satoshi Murakami, Tsuyoshi Inoue, Yusuke Mori.

### P-M037

The Development of a Unified Microfluidic Technology for High Throughput Protein Crystallization. Jiang Huang.

### P-M038

X-ray Evaluation of Undisturbed Protein Crystals in Crystallization Drops. Tadeusz Skarzynski.

### P-M039

Microseed Matrix Screening High-

Throughput Crystallization of Antibody Fabs and Fab/Antigen Complexes. Galina Obmolova, Thomas Malia, Alexey Teplyakov, Raymond Sweet, Gary Gilliland.

### P-M040

The Use of Tryptophan in Structural Genomics. Harindarpal S. Gill.

### P-M041

ProSeed: A General Method to Introduce Beneficial Nuclei to Promote Protein Crystallization. Jeff Habel. Li-Wei Hung

### P-M042

Structural Studies of Heme P460 in Hydroxylamine Oxidoreductase. Carrie Wilmoth, Peder Cedervall, Alan Hooper.

### P-M043

Structural Determinants for the Product Specificity of the Protein Methyltransferase SET7/9. Paul Del Rizzo, Jean-Francois Couture, Bethany Strunk, Marijo Roiko, Raymond Triebel.

### P-M044

Structural Insights into the Specificity and Adaptability of Near Germline Antibodies. Cory Brooks, Sven Müller-Leonnies, Lore Brade, Tomoko Hirma, Roger MacKenzie, Paul Kosma, Helmut Brade, Stephen Evans.

### P-M045

Crystallographic Studies on IDH from *Bacillus subtilis*. Karin Van Straaten, David Sanders, David Palmer.

### P-M046

Structural Investigations into the Digestion of Resistant Starch Structures by a Prominent Human Gut Microin. Jenny-Lyn Jacobs, David Rose.

### P-M047

Human Blood Group Glycosyltransferase Cysteine to Serine Mutants Reorder the Active Site Without Significantly Affecting Enzyme Activity. Stephen Evans, Brock Schuman, Mattias Persson, Roxanne

Landry, Robert Polakowski, Svetlana Borisova, Nina Seto, Monica Palcic.

**P-M048**

Structure of Carbohydrate Oxidase from *Microdochium nivale* in the Unliganded and Liganded Form. Jarmila Duskova, Jan Dohnalek, Tereza Skalova, Lars Ostergaard, Claus Fuglsang, Petr Kolenko, Andrea Stepankova, Jindrich Hasek.

**P-M049**

Structural Basis for the Recognition of Liparabinomannan by the Fab Fragment of the CS-35 Monoclonal Antibody. Tomohiko Murase, Ruixiang Blake Zheng, Maju Joe, Yu Bai, Sandra L. Marcus, Todd Lowary, Kenneth K.S. Ng.

**P-M050**

ZEEMANS - A High Magnetic Field Neutron Scattering Instrument. Andrei Savici, Garrett Granroth, Collin Broholm, Young Lee, Mark Bird.

**P-M052**

Garnet Geochemistry in Aliabad Cu-porphyr Skarn (Yazd), Central Iran. Batoul Taghipour, Mohamad Ali Mackizadeh, Arthur Kasson.

**P-M053**

*Melanocarpus albomyces* Laccase Complex with 2,6-dimethoxy Phenol Reveals two Catalytic Amino Acids in the Substrate-binding Pocket. Juha Kallio, Nina Hakulinen, Juha Rouvinen.

**P-M054**

RasMol to PyMOL Scripting Language Conversions. Scott Mottarella, Brett Hanson, Charles Westin, Paul Craig, Herbert Bernstein.

**P-M055**

Molecular-level Investigation of Single-crystal Monosodium Urate: Topography, Growth, and Chemical Interactions. Clare Yannette, Jennifer Swift.

**P-M056**

Use of the Next Generation Dictionary Definition Language, DDLm, in CIF validation with CBFlib. Elena Zlateva, Herbert Bernstein, Nikolay Darakev, Gregory McQuillan, Jonathan Ihm.

**P-M057**

New Molecular Graphics Movie Scripting Features under SBEVSL. Nikolay Darakev, Herbert Bernstein, Jonathan Ihm, Gregory McQuillan, Elena Zlateva, Paul Craig, Laura Grell.

**P-M058**

A Novel Method for Attenuating X-ray Damage to Protein Crystals. Kristopher White, Irimpan Mathews.

**P-M061**

Using the Cambridge Crystallographic Database to Aid the Study of Methanol and Dimethylsulphoxide Solvates. Monika Brychczynska, Davey Roger.

**P-M062**

Polymorphism from a Solution Perspective: Rationalisation at the Molecular Level. Vicky Fawcett, Guy Hembury, James McCabe, Sven Schroeder, Roger Davey.

**P-M063**

Crystal Structure of Co(II)diisopropylisonicotinamide Coordination Networks: Combination of Metal-ligand Coordination and Hydrogen Bonding to Self Assemble 3D Supramolecular Frameworks. Ajay Pal Singh Pannu, Maninder Singh Hundal, Ramesh Kapoor, Pratibha Kapoor.

**P-M064**

Impurity Effects on the Crystalline Habit of Pharmaceutical Substances. Kevin Back, Roger Davey, Stephen McGhie.

**P-M065**

Polytypism in Kettnerite. Jiri Hybler, Slavomil Durovic.

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### P-M066

Crystal Structure of 2,2,8,8-tetramethyl 3H,4H,9H,10H-benzo[c,h]dipyran-[a,j] Phenazine. Claudia Candida Silva, Janaina G. Ferreira, Regina Helena de Almeida Santos, Antonio Ventura Pinto.

### P-M067

Structural Analysis of the Thiourea  $C_{26}H_{22}N_4O_2S_2$ . Carlito Lariucci, Rodrigo Marinho, Hamilton Napolitano, Silvio Cunha.

### P-M068

Time-Resolved Photocrystallographic Investigation of Metastable Species. Mark Warren, Teresa Savarese, Stefanie Schiffers, Simon Brayshaw, Paul Raithby, Zoltan Gal.

### P-M069

The Structure of 2-(naphthyl)-3-pyridinyl-1,3-thiazolidin-4-one. Jose Pinto, Jose Nenaio, Diego Amado, Vladimir Kouznetsov, Teresa Gonzalez, Alexander Briceño.

### P-M070

Low Temperature Study of Diethylcarbamazine Citrate. Cecilia da Silva, Sara Honorato, Alejandro Ayala, Jorge Mendonça, Javier Ellena.

### P-M071

Cover That Structure: Some Results Selected by Journals for Their Front Covers and Other Illustrations. Luca Russo, William Clegg, Ross W. Harrington.

### P-M072

Intermolecular Interaction-directed Conformations of Bridged bis(1,4-piperazine-2,5-diones). Gary S. Nichol, Nathan W. Polaske, Lajos Z. Szabo, Bogdan Olenyuk.

### P-M073

Stable Five-Coordinate Trisboryl Analogs of Proposed Reactive Intermediates in Ir-Mediated C-H Borylations. Britt A. Van-chura II, Milton R. Smith III.

### P-M074

New Cyclopalladated Complexes of Benzylideneaniline with Different Bridging Ligands. Janaina G. Ferreira, Regina Helena A. Santos, Anderson M. Santana, Antonio Carlos Moro, Adelino V. Godoy Netto, Antonio Eduardo Mauro.

### P-M076

Er and Yb Complexes: Potencial Emissive Layers for OLEDs. Manuela Ramos Silva, Pedro S. Pereira Silva, Pablo Martin-Ramos, Ana Matos Beja, Jose A. Paixao, Jesus Martin-Gil.

### P-M077

Crystal Structures and NLO Properties of Salts with Octupolar and 2-Dimensional Chromophores. Pedro Pereira Silva, Manuela Ramos Silva.

### P-M078

Supramolecular Networks of Organically Templated Transition Metal Sulfates. Houcine Naili, Walid Rekik, Tahar Mhiri, Thierry Bataille.

### P-M079

0D, 1D and 2D Organically Templated Transition Metal Sulfates: Crystal Structure, Thermal Behaviour and Magnetic Properties. Ahmed Bakir, Houcine Naoli, Walid Rekik, Tahar Mhiri, Thierry Bataille.

### P-M080

Co-crystals of 1,3-adamantanedicarboxylic Acid with Some Aza-donor Compounds. Yogesh Manjare, V. R. Pedireddi.

### P-M081

Perylene Crystallization on 2-D Templates. Jessica Urbelis, Jennifer A. Swift.

### P-M082

Co-crystallising Agents for the Assembly of Binary and Ternary Co-crystals. Sheelu Panikkattu, Christer Aakeroy, John Desper.

**P-M083**

N-oxides as a Ready Tool for Organic Co-crystals. Abhijeet Sinha, Christer Aakeroy, John Desper.

**P-M084**

Supramolecular Structure and a New Malaria Pigment Model System. Ratchadaporn Puntharod, Kenneth Haller, Grant Webster, Mehdi Asghari-Khiavi, Keith Bambery, Bayden Wood.

**P-M085**

Probing Hydrogen-bonding and Halogen-bonding in the Solid-State using Halogenated Pyrazoles and Carboxylic acids. Evan Hurley, Christer Aakeroy, John Desper.

**P-M086**

Topological Diversity in Pillared Porphyrin Frameworks. Haemi Chung, Paul Barron, Richard Novotny, Hyun-Tak Son, Chunhua Hu, Wonyoung Choe.

**P-M087**

Concerted Aryl Interactions in Zinc-Imidazole Complex Hybrid Oxovanadates. Samroeng Krachodnok, Kenneth J. Haller, Ian D. Williams.

**P-M088**

Co-crystals: A New Dawn in Pharmaceutical Research. Naheed Haque, Christer Aakeroy, John Desper.

**P-M089**

Crystallography and Imaging: Towards Bridging the Gap in the Structural Biology. Elizabeth Duke.

**P-M090**

Bragg Surface Diffraction as a Probe for Studying InAs/GaAs Free-Standing Quantum Dots Systems. Raul Freitas, Stefan Kyrcia, Alain Quivy, Sergio Moreleo.

**P-M091**

Crystal Structure and Functional Assay of the N-acetylglucosamine-1-phosphate Uri-

dyltransferase from *Mycobacterium tuberculosis*. Jiang Yin, Craig Garen, Maia Cherney, Leonid Cherney, Michael James.

**P-M092**

New Insights Into the Activation Of G Proteins: Crystal Structure Of A Constitutively Active Mutant Transducin. Garima Singh, Richard A. Cerione.

**P-M093**

Opportunities for Structure-based Design of Calpain Inhibitors. Kristin E. Low, Rachel A. Hanna, Jacqueline Kelly, Robert L. Campbell, Peter L. Davies.

**P-M094**

Thermofluor-Based Approach to Fragment Screening of HIV-1 Reverse Transcriptase. Disha Patel, Joseph Bauman, Chhaya Dharria, Arthur Clark, Eddy Arnold.

**P-M095**

Structural Studies of Acid  $\beta$ -Glucosidase in Complex with Pharmacological Chaperones. Susan Orwig, Raquel Lieberman.

**P-M096**

Polymorphism of a N-Benzoyl-Guanidine: 4-Methoxy-1-[4-methoxyanilino(phenylcarbonylimino)-methylamino]benzene. Hamilton Napolitano, Carlito Lariucci, Ademir Camargo, Silvio Cunha.

**P-M097**

The Crystal Structure of the Fusion Protein, Orotidine Monophosphate Decarboxylase - Orotate Phosphoribosyl Transferase from *Leishmania donovani*. Jarrod B. French, Buddy Ullman, Steven E. Ealick.

**P-M098**

Hydrogen-bond Patterns in the 1,3,6-cyclohexanopentol. Paulo Junior Carvalho, Hamilton B. Napolitano, Ademir J. Camargo.

**P-M099**

SrRietveld: A Python Application for Au-

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tomating FullProf and GSAS Rietveld Refinements. Peng Tian, Wenduo Zhou, Pavol Juhas, Emil Bozin, Christopher Farrow, Simon Billinge.

### P-M100

Protein Crystal Imaging with the Detect-X Microscope. Peter Nollert, Werner Kaminisky, Timothy Vincent, Chad Warren, Mark Mixon.

### P-M101

Providing "Light When YOU Need It" via SER-CAT's Virtual Synchrotron. John Chrzas, James Fait, John Gonczy, Zhongmin Jin, Zheng-Qing Fu, Andrew Howard, John P. Rose, Bi-Cheng Wang.

### P-M102

Optics for Macromolecular Crystallography (MX) Beamlines Being Planned for NSLS-II. Howard Robinson, Lonny Berman, Robert Sweet, Dieter Schneider, Marc Allaire, Mark Chance, Mike Sullivan, Allen Orville, Vivian Stojanoff, Wayne Hendrickson.

### P-M103

NorthEastern Collaborative Access Team (NE-CAT) Beam Lines at the Advanced Photon Source. Igor Kourinov, Steve Ealick, Malcolm Capel, Frank Murphy, David Neau, Kay Perry, Kanagalaghatta Rajashankar, Jonathan Schuermann, Narayanasami Sukumar.

### P-M104

New Capabilities at GM/CA CAT Beam Lines at the APS. Nagarajan Venugopalan, Mark Hilgart, Sudhir Babu Pothineni, Derek Yoder, Sergey Stepanov, Michael Becker, Ruslan Sanishvili, Craig Ogata, Janet Smith, Robert Fischetti.

### P-M105

Instrumentation for Micro-Crystallography at GM/CA-CAT. Robert Fischetti, Derek Yoder, Shenglan Xu, Oleg Makarov, Richard Benn, Sergey Stepanov, Nukri Sanishvili, S. Vogt, Janet Smith.

### P-M106

Unusual Te-Te interactions in New Barium Copper Selenide-Tellurides. Mayasree Oottil, Yanjie Cui, Abdeljalil Assoud, Holger Kleinke.

### P-M107

Structural and Thermoelectric Properties of the Chemically Doped Incommensurate  $\text{Ca}_3\text{Co}_4\text{O}_9$  System. Tao Wu, T. A. Tyson, Z. Chen, Q. Jie, Q. Li, J. J. Tu.

### P-M108

Lanthanide Metal-Organic Framework Materials: Structure and Properties. Ping-Yen Hsieh, Yun Liu, Robert M. Briber, Mark A. Green.

### P-M109

Carotenoid Cleavage in Plants: The Structure of the Membrane Penetrating VP14. Simon Messing, Sandra Gabelli, Ignacia Echeverria, Jonathan Vogel, Jiahn Chou Guan, Bao Cai Tan, Harry Klee, Donald McCarty, L. Mario Amzel.

### P-M110

Characterization of *Pseudomonas aeruginosa* PilF and its Role in Type IV Pilus Assembly. Jason Koo, Stephanie Tamman, Shao-Yang Ku, Tim Tang, Liliana Sampaianu, Lori L. Burrows, P. Lynne Howell.

### P-M111

Crystallization of TrbC from the *Escherichia coli* Type 4 Secretion Systems. Agnesa Shala, Gerald F. Audette.

### P-M112

Towards Crystallization of Nicotinamide Transhydrogenase. Mikael Ekvall, Susanna Tornroth-Horsefield.

### P-M113

Structural Determination of Agonist Behavior at Ionotropic Glutamate Receptors. Elizabeth Andrews, Gregory Miller, Derek Bowie.

**P-M114**

Physical Properties and Phase Changes in Scandium Fluoride. Kenneth L. Martin, Karena W. Chapman, Benjamin K. Greve, Peter L. Lee, Chad J. Ruschman, Angus P. Wilkinson.

**P-M115**

Structural Phase Transitions in Molecular Systems. Ross Angel, Maciej Bujak.

**P-M116**

Phase Transition of Copper Phthalocyanine. Juergen Graf, Carsten Michaelsen, Bernd Hasse, Melanie Mueller, Robert Dinnebier.

**P-M117**

A New Crystal Structure of  $\text{KHCO}_3$  and Phase Transitions Study. Chuttree Phurat, Nongnuj Muangsin.

**P-M118**

Structure and Phase Transitions of the Polymeric Organic-Inorganic Hybrids:  $[\text{M}(\text{imidazole})_4\text{V}_2\text{O}_6]_\infty$ , M = Mn, Co, Ni. Kenneth J. Haller, Kittipong Chainok, A. David Rae, Anthony C. Willis, Ian D. Williams.

**P-M119**

High-Density Hydrate Phases of Carbon Dioxide. Daniel Pohl, Jesse Smith, Serge Desgreniers.

**P-M120**

Pressure-induced Structural Phase Transition in the bis-1,2,3-thiaselenazolyl Radical Solid. Laura Downie, Serge Desgreniers, John Tse, Richard Oakley.

**P-M121**

Case Studies on Polymorphism: Crystallization, Structures and Solid-state Properties. Alicia Ng, Qi Gao, Chiajen Lai, Feng Qian, Baoqing Ma.

## Tuesday Posters

### P-T001

Novel Fold of VirA, a Type III Secretion System Effector Protein. Jamaine Davis, Jiawei Wang, Di Zhang, Joseph Tropea, Zbigniew Dauter, David Waugh, Alexander Wlodawer.

### P-T002

Advantage of 3D Single Reflection Optics for Small Protein Crystal and Long Unit Cell Analysis. Vincent Roger, Blandine Lantz, Sergio Rodrigues.

### P-T003

Structural and Enzymatic Properties of a Trimeric Adenylate Kinase from the Mesophile *Methanococcus maripaludis*. Milya Davlieva, Yousif Shamoo.

### P-T004

X-ray Structural Studies on the N-domain of the Wilson Disease Associated Protein. Sean Dalrymple, Lata Prasad, Lili Liu, Christopher O'Grady, Oleg Dmitriev, Louis Delbaere.

### P-T005

Crystal Structure of the N-terminal Domain of Mast/Orbit from *Drosophila Melanogaster*. Teresa De la Mora-Rey, Brian Guenther, Barry Finzel.

### P-T006

A New Approach to Identification of Surface Residues. Herbert J. Bernstein, Paul A. Craig.

### P-T007

Crystal Structures of the Effector Protein "Cif" from Two Bacterial Pathogens. Mark Banfield, Paul Race, Gregory Jubelin, Carolina Varela-Chavez, Jean-Michel Escoubas, Eric Oswald, Allister Crow.

### P-T008

Three-dimensional Structure and Functional Annotation of the Protein Dr0930

from *Deinococcus radiodurans*. Alexander Fedorov, Elena Fedorov, Dao Feng Xiang, Frank Raushel, Steve Almo.

### P-T009

Complete Neutron Laue Data Collection at 293K on a Perdeuterated 'tiny' Crystal of Type III Antifreeze Protein. Andre Mitschler, Blakeley Matthew, Petit-Haertlein Isabelle, Mueller-Dieckmann Christoph, Popov Alexandre, Howard Eduardo, Haertlein Michael, Podjarny Alberto.

### P-T010

Structures of Protein Farnesyltransferase and Protein Geranylgeranyltransferase-I from the Human Fungal Pathogen *Candida albicans*. Michael Hast, Lorena Beese.

### P-T011

Crystal Structure of Human Exonuclease I Catalytic Domain with DNA Substrate. Jillian Orans, Elizabeth McSweeney, Paul Modrich, Lorena Beese.

### P-T012

Crystal Structure of Fosfomycin Resistance Kinase FomA. Svitlana Pakhomova, Sue Bartett, Alexandria Augustus, Marcia Newcomer.

### P-T014

Crystal Structures and Multi-conformer Refinement of 70S Ribosome Translation Termination Complexes Formed with Release Factors RF1 and RF2. Andrei Korostelev, Haruichi Asahara, Laura Lancaster, Martin Laurberg, Jianyu Zhu, Sergei Trakhanov, Alexander Hirschi, William Scott, Harry Noller.

### P-T015

High-Resolution Structure of Barrier to Autointegration Factor (BAF): A Host Factor for Retrovirus and Poxvirus Replication. Timothy Umland, William Bauer.

**P-T016**

Crystal Structures of Phosphorylation-site Mutants of the KaiC Circadian Clock Protein and Mechanisms of the Kinase and ATPase Activities. Rekha Pattanayek, Yao Xu, Tet-suya Mori, Carl Johnson, Martin Egli.

**P-T017**

The Structure and Function of NudC. Urszula Derewenda, Meiyang Zheng, Alexander J. Burdette, Kim A. Caldwell, Pawel Janczyk, P. Todd Stukenberg, Zygmunt S. Derewenda.

**P-T018**

Crystal Structure and Functional Characterization of DNA Damage Response B from the Radiation Resistant Thermophile *Deinococcus geothermalis*. Seiji Sugiman-Marangos, Murray Junop.

**P-T019**

Structural Studies of JlpA, a Surface Exposed Lipoprotein from *Campylobacter jejuni*. Hye-Jeong Yeo, Seonghee Paek, Fumihiko Kawai, Patricia Guerry.

**P-T020**

Studying the Evolution of an Archaeal Membrane Lipid-Synthesizing Enzyme: (S)-3-O-Geranylgeranylglycerol Phosphate Synthase (GGGPS). Neha Kharbanda, Jian Payandeh, Emil F. Pai.

**P-T021**

Conformational Determinants of Phosphotyrosine Peptides Complexed with the Src SH2 Domain. Joseph Nachman, Gerry Gish, Cristina Virag, Tony Pawson, Regis Pomes, Emil Pai.

**P-T023**

MacCHESS 2009. David J. Schuller, Rick Cerione, Ulrich Englisch, Richard Gillilan, Sol Gruner, Xinguo Hong, Chae Un Kim, Qun Liu, D. Marian Szebenyi, M. Cook, I. Kriksunov, W. Miller, S. Smith.

**P-T024**

Making Sense of Macromolecular Refinement Restraints. Mark White.

**P-T025**

Analysis of HIV-1 Protease Variants with Engineered Disulfide Bonds to Support Hydrophobic Core Sliding as a Possible Mechanism for its Enzymatic Activity. Seema Mittal, Celia A. Schiffer.

**P-T026**

Structure and Inhibition of *E. coli*  $\beta$ -Glucuronidase: Improving Anticancer Drug CPT-11 Efficacy. Bret Wallace, Kimberly Lane, John Scott, Li-An Yeh, Matthew Redinbo.

**P-T027**

Functional and Structural Analysis of the LysR Family Transcriptional Regulator AmpR. Misty Balcewich, Brian Mark.

**P-T028**

Coevolution of Plant Shikimate Kinase Fold and Gene Expression. Geoff Fucile, Dinesh Christendat.

**P-T029**

The PDB: Updates and Future Plans. Martha Quesada, Jasmine Young, Shuchismita Dutta, Zukang Feng, John Westbrook, Dimitris Dimitropoulos, Miri Hirshberg, Jawahar Swaminathan, Kim Henrick, Takanori Matsuura, Haruki Nakamura, Joh Markley, Helen M. Berman.

**P-T030**

X-ray Radiation Induced Co-operative Atomic Movements in Protein. Andrzej Joachimiak, Tatiana Petrova, Vladimir Lunin, Stephan Ginell, Isabelle Hazemann, Krzysztof Lazarski, Andre Mitschler, Alberto Podjarny.

**P-T031**

Slow Cooling of Protein Crystals: A New Approach for Low- and Variable-temperature Crystallographic Data collection. Mat-

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thew Warkentin, Robert Thorne.

### P-T032

The Structural Biology Center User Program at the Advanced Photon Source, Argonne National Laboratory. Stephan Ginell, Randy A. Alkire, Changsoo Chang, Marianne E. Cuff, Norma E. C. Duke, Kazimierz Gofron, Youngchang Kim, Krzysztof Lazarski, Jack Lazarz, Mike Molitsky B. Nocek, J. Osipiuk, S.O. Park, G. Rosenbaum, F.J. Rotella, K. Tan, R-g. Zhang, A. Joachimiak.

### P-T033

Crystal Structure of *Pseudomonas fluorescens*-encoded Superantigen pflT. Hongmin Li, Lihui Liu, Guo Yi.

### P-T034

Investigating the Autoinhibitory Mechanism of IP6K2. Varin Gosein, Gregory J. Miller.

### P-T035

The Structural Basis for Recognition of the PreQ0 Metabolite by an Unusually Small Riboswitch Aptamer Domain. Joseph Weidekind, Robert Spitale, Andrew Torelli, Jolanta Krucinska, Vahe Bandarian.

### P-T036

The Structural Basis of Double-Stranded RNA Recognition by the RIG-I like Receptor MDA5. Xiaojun Li, Cheng Lv, Mikela Nelson, Tatyana Igumenova, Pingwei Li.

### P-T037

The Structures of the Catalytic Domain of Human Receptor-Like Protein Tyrosine Phosphatase gamma in Three Different Conformations. Steven Sheriff, Brett Beno, Patrica McDonnell, Kevin Kish, Valentina Goldfarb, Mian Gao, Susan Kiefer, David Langley, Yanling Huang, Samuel Gerritz, Weixu Zhai, Shirong Zhu, Shuhao Shi, Carolyn Dzierba, Kingsley Appiah, Ryan Westphal, Jonathan O'Connell, Walter Kostich.

### P-T038

The Crystal Structure of the Arginine Repressor Protein from *Mycobacterium tuberculosis* Bound with its DNA Operator. Maia Cherney, Leonid T. Cherney, Craig R. Garen, George J. Lu, Michael MN James.

### P-T039

Absence of a Catalytic Water Confers Resistance to the Neurotoxin Gabaculine. Joerg Stetefeld, George Orriss, Trushar Patel.

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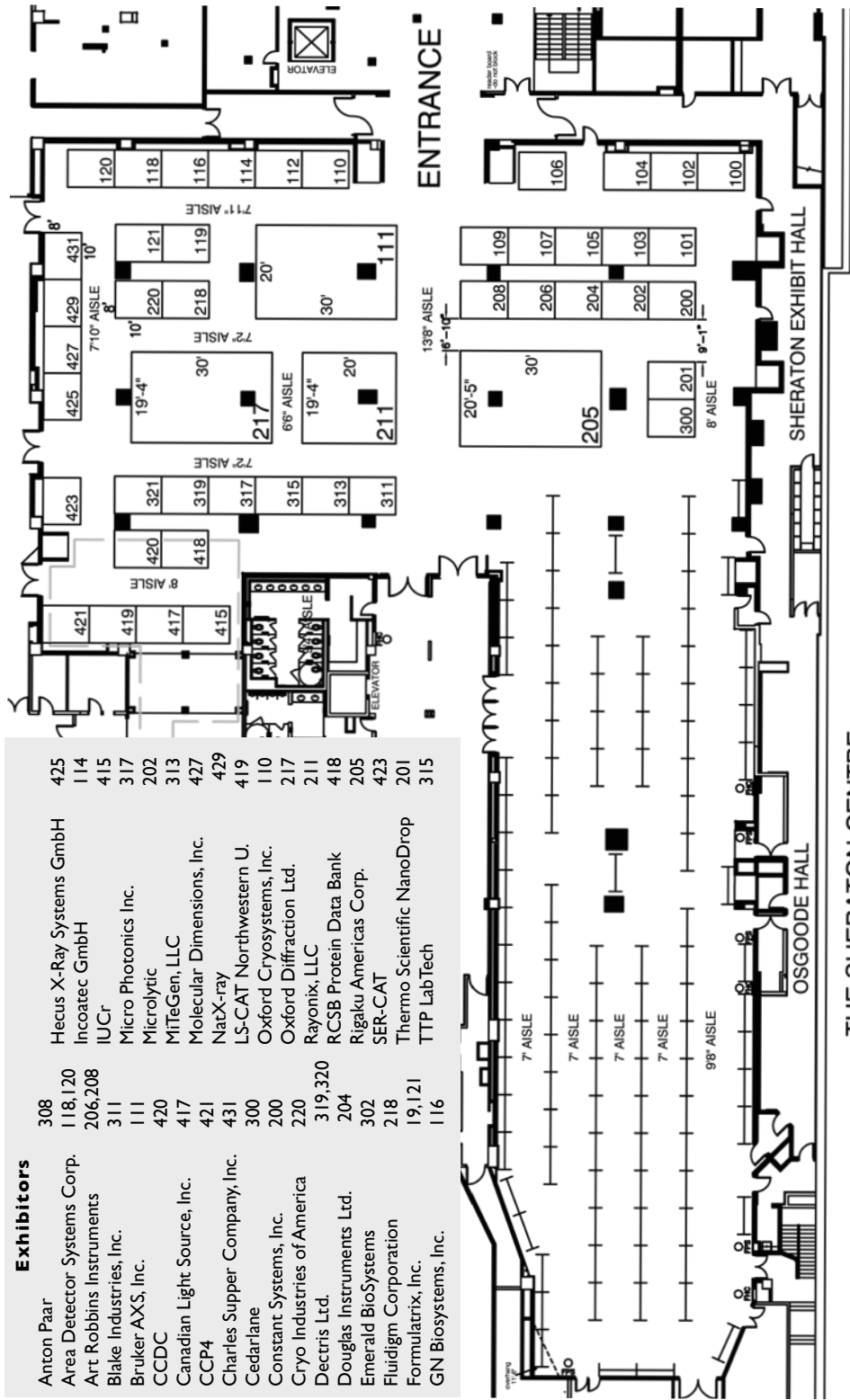


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