ANNUAL MEETING

May 28 - June 2, 2011
New Orleans, LA

Program

www.AmerCrystalAssn.org
American Crystallographic Association
2011 Annual Meeting
May 28 - June 2
New Orleans, LA

Program Chair: Chris Cahill
Local Committee: Cheryl Stevens, Ed Stevens, Frank Fronczek
Poster Chair: Ilia Guzei

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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.
**SATURDAY, MAY 28**

**WK.01 Symmetry-mode Analysis**
Chair: Branton Campbell
Maurepas

**08:00-08:30am Introduction to symmetry-mode analysis (M. Perez-Mato)**
- Distortions and their order parameters (strain, displacive, occupational, magnetic).
- Symmetry modes are a relative description that depends on the parent structure.
- Irreps of the parent symmetry and their basis functions.
- Irrep basis functions provide a symmetry-motivated basis for distortions.
- Define distortion symmetry and isotropy subgroup (single-irrep distortion).
- Irrep coupling to get more complicated distortions.

**08:30-10:00am Exploring structural distortions with ISODISTORT (B. Campbell and H. Stokes)**
- Distortion output:
  - Distortion symmetry – specifies space-group type, origin and basis
  - Visualization tools, CIF, mode details, primary OPs, domains, other
- Filtered search tools for generating distortion models:
  - Database search – commensurate single-irrep distortions
  - Search by supercell and space-group type
  - Search by k-point/irrep/OPD
- Domains
- Primary vs secondary order parameters
- Coupled order-parameters
- Incommensurate example and super-space-symmetry

10:00-10:30am  Coffee break

**10:30-12:00pm Symmetry mode analysis with AMPLIMODES & FULLPROF (M. Perez-Mato)**
- Define mode amplitudes
- Mode-decomposition examples
- Order-parameter evolution near a phase transition and critical exponents
- Symmetry-mode refinement(s) using Fullprof

12:00-01:00pm  Lunch break

**01:00-02:30pm Symmetry-mode analysis with ISODISTORT & TOPAS (B. Campbell and H. Stokes)**
- Work through mode decomposition examples
- Work through symmetry-mode refinement(s) using TOPAS
- How to “solve” a distorted structure on the symmetry-mode basis

**02:30-03:00pm Magnetic symmetry (H. Stokes)**
- Review magnetic symmetry and nomenclature
- Walk users through the online magnetic-symmetry database
- The relationship between the OG and BNS settings
- How to describe a magnetic structure
- The relationship between the OG and BNS settings

**03:00-03:30pm Coffee break**

**03:30-04:30pm Magnetic distortions (M. Perez Mato)**
- Introduce magnetic distortions
- Examples using ISODISTORT
- An incommensurate magnetic distortion

**04:30-05:00pm Magnetic symmetry-mode refinement (B. Campbell)**
- A magnetic refinement using TOPAS
- Many magnetic structures are “solved” now in P1. Emphasize utility of mag symmetry
WK.02 Introduction to PHENIX for Beginning to Advanced Crystallographers
Chair: Paul Adams Borgne

08:30am  PHENIX Overview (Paul Adams)
08:50am  Automation of Structure Determination in PHENIX (Tom Terwilliger)
09:35am  Break and set-up of PHENIX on individual computers
10:00am  Molecular Replacement (Paul Adams)
10:45am  Refinement with X-rays and neutrons in PHENIX (Pavel Afonine)
11:30am  Structure Validation (Chris Williams)
12:15pm  Lunch break
01:00 - 02:00pm  Group Tutorial -- Data analysis and Structure solution
02:00 - 03:00pm  Group Tutorial -- Model-building and Ligand Fitting
03:00 - 03:30pm  Coffee break
03:30 - 04:30pm  Group Tutorial -- PHENIX Refinement and Validation

New Student Orientation
06:30pm  D1
Chair: Eric Armstrong
The focus of this informal session is to orient ‘young scientists’ and first time attendees to the structure of the ACA Meeting and how to make the most of their experience.

Opening Reception
Exhibit Show and Presidential Welcome
07:30pm  Napoleon Ballroom
SP.01 2011 Margaret C. Etter Early Career Award
Chair: Jamaine Davis
D2-D3
Award presentation to Yurij Mozharivskyj by President Thomas Koetzle.

08:00am-08:50am SP.01.1

SP.01 Etter Early Career Award Symposium
Chair: Jamaine Davis
D2-D3

09:00-09:20am SP.01.2 Spy: a New Class of Molecular Chaperones. Karen Ruane, Shu Quan, James C.A. Bardwell, Rong Shi, Miroslaw Cygler.


09:40-10:00am SP.01.4 Detergent, Bicelle, and LCP Crystallization of the Outer Membrane Protein intimin from Enterohemorrhagic E. coli (EHEC). James Fairman, Travis Barnard, Nicholas Noinaj, Susan Buchanan.

10:00-10:30am Coffee break

10:30-10:50am SP.01.5 Structural Insights Into the Role of Protein Surface Flexibility in the Regulation of Polo-Like Kinase 1. Pawel Sledz, Steffen Lang, Christopher Stubbs, Grahame McKenzie, Ashok Venkitaraman, Marko Hyvonen, Chris Abell


11:05-11:20am SP.01.7 Structure of the Human RON Receptor Tyrosine Kinase in Complex With the MSP β-Chain. Kinlin Chao, I-Wei Tsai, Natalia Gorlatova, Chen Chen, Osnat Herzberg.

11:20-11:40am SP.01.8 Crystal Structure of a Clade C HIV-1 gp120 Bound to Cd4 and Cd4-Induced Antibody. Ron Diskin, Paola Marcocvecchio, Pamela Bjorkman.

11:40-12:00pm SP.01.9 Crystal Structure of Human Dual-Specificity Phosphatase 27, An Atypical DUSP. George Lountos, Joseph Tropea, David Waugh.
01.01 Use of Databases in Structural Biology
Chair: Wladek Minor

09:00-09:30am  01.01.1
Putting the "Data" in "Data Mining": Curating the PDB Archive. Helen Berman, Gerard Kleywegt, Haruki Nakamura, John Markley.

09:30-10:00am  01.01.2
Biomolecular Interactions: a New Look at NCBi's Structural Biology Information Resources. Stephen Bryant.

10:00-10:30am  Coffee break

10:30-11:00am  01.01.3

11:00-11:30am  01.01.4
Protein Structural Similarity: Tools, Databases, and Problems. Adam Godzik.

11:30-11:50am  01.01.5

11:50-12:00pm  01.01.6
Using Small Molecule Crystal Structure Data for Ligands in Protein-Complex Structure Determination. Thomas Womack, Gerard Bricogne, Claus Flensburg, Peter Keller, Wlodek Padiorek, Andrew Sharff, Clemens vonrhein, Oliver Smart.

12:10-12:30pm  01.01.7
Enhancements to the LabDB Crystallographic Laboratory Information Management System. Matthew Zimmerman, Kamila Wojciechowska, Wojtek Wajerowicz, Zbigniew Fratczak, Wladek Minor.

02.01 General Interest I
Chair: Peter Mueller
Maurepas

09:00-09:15am  02.01.1

09:15-09:30am  02.01.2
Resolution of Racemic Pharmaceuticals Via Crystallization on Chiral Templates. John MacDonald, Pranoti Navare.

09:30-09:45am  02.01.3

09:45-10:00am  02.01.4
New Models in Mathematical Crystallography. Olga Smirnova.

10:00-10:30am  Coffee Break

10:30-11:00am  02.01.5
Lee-Richards Surfaces, Gaussians and Nearest Neighbors. Herbert J. Bernstein, Lawrence C. Andrews.

11:00-11:30am  02.01.6

11:30-12:00pm  02.01.7
08.01 In situ Diffraction Studies
Chairs: Christine Beavers, Craig Bridges
D1

09:00-09:25 08.01.2

09:25-09:45am 08.01.3
Structural and Magnetic Properties of Cobalt Oxide Under Pressure. Antonio dos Santos, Jamie Molaison, Christopher Tulk, Yansun Yao, Dennis Klug.

09:45-10:00am 08.01.4
Expanding the Power of High Resolution Powder Diffraction; in-situ Studies at 11-Bm. Matthew Suchomel, Lynn RibaudArgonne National Laboratory, Haiyan Zhao, Mathieu Allix.

10:00-10:30am Coffee Break

10:30-10:55am 08.01.5
Light and Pressure Induced Solid-State Transformations in Dithienylethenes and Their Metal Complexes. Paul Raithby, Simon Brayshaw, Christopher Woodall, Stefanie Schiffer, Anna Stevenson, Mark Warren, David Allan, John Warren, Julia Weinstein.

10:55-11:10am 08.01.6

11:10-11:35am 08.01.7

11:35-11:50am 08.01.8

11:50-12:00pm 08.01.9

04.01 Surfaces and Interfaces
Chair: Zhang Jiang & Masafumi Fukuto Maurepas

01:30-02:00pm 04.01.1

02:00-02:20pm 04.01.2
Screening Effect of Highly Compressible Supercritical Carbon Dioxide on Attractive Polymer/Substrate Interactions. Tad Koga, Peter Gin, Naisheng Jiang, Maya Endoh, Bu-lent Akgun, Sushil Satija.

02:20-02:40pm 04.01.3

02:40-03:00pm 04.01.4

03:00-03:30pm Coffee Break

03:30-04:00pm 04.01.5
Surfaces Sensitive and Ion-Specific X-Ray Spectroscopy and Diffraction at Liquid Interfaces. David Vaknin.

04:00-04:30pm 04.01.6
04:30-05:00pm 04.01.7

08.02 Structural Enzymology I: Spectroscopy and Complementary Methods
Chair: Allen Orville Borgne
01:30-02:00pm 08.02.1

02:00-02:30pm 08.02.2
This Side Or the Other? Selective Cleavage at the S-Adenosylmethionine Sulfur Atom by a Radical [4Fe-4S]-Containing Enzyme. Andrew Torelli, Yang Zhang, Xuling Zhu, Hening Lin, Steven E. Ealick.

02:30-03:00pm 08.02.3

03:00-03:30pm Coffee Break

03:30-04:00pm 08.02.4
Insights Into the Mechanism of Heme Degradation by the Isdg-Like Family of Enzymes. Michael Murphy, Georgia Ukpabi, Sarah Thackray.

04:00-04:30pm 08.02.5

04:30-05:00pm 08.02.6
Defining the Role of the Axial Ligand of the Type 1 Copper Site in Amicyanin, An Electron Transfer Protein from Paracoccus denitrificans. Narayanasami Sukumar, Moonsung Choi, Victor Davidson.

08.03 Crystallography and the Search for New Materials
Chair: Svilene Bobev
D1
sponsored, in part, by Agilent Technologies, Bruker AXS, Inc., and Rigaku Americas Corp.

01:30-01:55pm 08.03.1

01:55-02:15pm 08.03.4

02:15-02:35pm 08.03.6

02:35-03:00pm 08.03.8

03:00-03:30pm Coffee Break

03:30-03:55pm 08.03.9
03:55-04:15pm 08.03.11

04:15-04:35pm 08.03.12

04:35-05:00pm 08.03.13
Conventional and Unconventional Crystallographic Investigations Into Materials for Photocatalysis and Other Energy Applications. Peter Khalifah.

08.04 Scholarly and Pragmatic Aspects of Crystallographic Publication Practices
Chairs: Larry Falvello & Ilia Guzei
D2-D3
sponsored, in part, by Agilent Technologies, Bruker AXS, Inc., and International Union of Crystallography

01:30-01:55pm 08.04.1

01:55-02:15pm 08.04.2

02:15-02:40pm 08.04.3
CheckCIF and CIF in a Multi-User Crystallography Facility. Richard Cooper.

02:40-03:00pm 08.04.4
Structure Validation and Manuscript Preparation with Apex2. Bruce C. Noll, Charles F. Campana, Kaercher Joerg.

03:00-03:30pm Coffee Break

03:30-03:50pm 08.04.5
### SP.02 Plenary Lecture:
**Philip Coppens, University of Buffalo**

**D2-D3**

08:00-08:50am  
From the Sun to Femtosecond Lasers and Back: Photo-Induced Dynamic Processes in Solids.

### 01.02 Protein Structure Initiative: Tools for the Home Lab
**Chair:** Ward Smith  
**Borgne**

09:00-09:20am  
High-Throughput Crystallization Screening for the Structural Biology Community. Michael Malkowski, Eleanor Cook, Mary Koszelak-Rosenblum, Angela Lauricella, Raymond Nagel, Elizabeth Snell, Jennifer Wolfley, Edward Snell, Joseph Luft, George DeTitta.

09:20-09:40am  

09:40-10:00am  

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

10:30-10:50am  
**01.02.4**  

10:50-11:10am  
**01.02.5**  

11:10-11:30am  
**01.02.6**  
Using the PSI: Biology-Materials Repository: a Biologist’s Resource for Protein Expression Plasmids. Catherine Cormier, Jin Park, Michael Fiacco, Jason Steel, Jason Kramer, Preston Hunter, Rajeev Singla, Joshua LaBaer.
MONDAY, MAY 30

04.02 Small Angle Scattering From Colloids
Chair: Gregory Beaucage & P. Russo
D1

09:05-09:30am 04.02.1 Structural Changes in BP Crude Oil During Degradation. Henning Lichtenberg, Amitava Roy, Edward Overton.

09:30-09:55am 04.02.2 Capillary Interactions in Nano-Particles Suspensions. Dobrin Bossev.

10:00-10:30am Coffee break


11:45-12:00pm 04.02.6 A Study of the Supramolecular Properties of Meso-Tetra(4-Sulfonatophenyl)Porphyrin in Aqueous Solutions. Javor’s Hollingsworth, Paul Russo, Allison Richard, Graca Vicente.

08.07 Materials for a Sustainable Future
Chairs: Ashfia Huq & Claudia Rawn
Maurepas

09:00-09:30am 08.07.1 The Search for Rapid Pathways to Synthesize CnlnxGa1-xSe2 Thin Film PV Absorbers. Tim Anderson, Ranga Krishnan, Christopher Muzzillo, Woo Kyoung Kim, Andrew Payzant, Carelyn Campbell, Jianyun Shen.

09:30-10:00am 08.07.2 Phase Transitions in Cu-Sb-Se and Ag-Mg-Sb Thermoelectric Materials. Melanie Kirkham, Antonio Moreira Dos Santos, Claudia Rawn, Jeff W. Sharp, Alan J. Thompson, Paul Majsztik, Eric Skoug, Donald Morelli, E. Andrew Payzant, Edgar Lara-Curzio.

10:00-10:30am Coffee Break

10:30-11:00am 08.07.3 Causes of Ion Selectivity in Porous Silicates. Aaron Celestan, Samantha Kramer, Kristin Leftwich.

11:00-11:20am 08.07.4 Structural Changes of the Type-I Clathrate Ba8AlxSi46-x (X = 8, 10, 12, 14, 16) Revealed by Neutron Powder Diffraction. John Roudebush, Clarina Dela Cruz, Bryan Chakoumakos, Susan Kauzlarich.


11:40-12:00pm 08.07.6 Visualization of Guest-Host Interactions in Energy Storage Materials Using X-Ray and Neutron Diffraction Methods. Xiaoping Wang, Chi Yang, Mohammad A. Omary, Bryan C. Chakoumakos, Huibo Cao, Abhijit
Pramanick, Christina Hoffmann.

12:00-01:30am Lunch Break.

01:30-02:00pm 08.07.7

02:00-02:20pm 08.07.8

02:20-02:40pm 08.07.9

02:40-03:00pm 08.07.10
In situ XRD of Li(Mn15Ni05)O4 Cathodes for Lithium Ion Batteries During Formation and Operation Cycles. Kevin Rhodes, Roberta Meisner, Yoongo Kim, Nancy Dudney, Claus Daniel.

03:00-03:30pm Coffee Break

03:30-04:00pm 08.07.11
Sr2Fe1.5Mo0.5O6-δ has Been of Interest as an Anode Material in Solid Oxide Fuel Cells. Hans-Conard zur Loye, Daniel Bugaris, Qiang Liu, Guoliang Xiao, Fanglin Chen.

04:00-04:20pm 08.07.12

04:20-04:40pm 08.07.13
Atomic Displacements and Thermal Motion in Triphylite-Lithiophilte, Li(Fe,Mn)Po4, Solid Solution. Bryan C. Chakoumakos, Xiaoping Wang, Huibo Cao.

04:40-05:00pm 08.07.14

MONDAY, MAY 30

TR.01 Transactions - Time-Resolved and Charge Density in Honor of Philip Coppens
Chair: Yu-Sheng Chen, Peter Lee
D2-D3
sponsored, in part, by Univ. of Chicago/CARS and Bruker AXS, Inc.

09:00-09:10am Introduction

09:10-09:40am TR.01.1
X-Ray Transient Absorption Spectroscopy: a Decade and Beyond. Lin Chen.

09:40-10:10am TR.01.2

10:10-10:30am Coffee Break

10:30-11:00am TR.01.3
Opto-Magnetic Switchable Character in Fe(II) Spin Crossover Complexes. Yu Wang, Chou-Fu Sheu, Che-Hsiu Shih, Masaki Takata.

11:00-11:30am TR.01.4

11:30-12:00pm TR.01.5

12:00-12:30pm TR.01.6
Time Resolved Laue Crystallography - Moving From 3Rd Generation Sources to Fel Experiments. Marc Messerschmidt.

12:30-01:30pm Lunch Break
Afternoon Chair: Jason Benedict

01:30-02:00pm  TR.01.7

02:00-02:30pm  TR.01.8

02:30-03:00pm  TR.01.9
Experimental Essentials for Charge Density Studies. Finn Krebs Larsen, Bo Iversen, Jacob Overgaard, Mette Schmoekel, Mads Ry Jørgensen.

03:00-03:30pm Coffee break

03:30-03:55pm  TR.01.10

03:55-04:20pm  TR.01.11
Within and Beyond the Pseudoatom Model. Tibor Koritsanszky.

04:20-04:40pm  TR.01.12

04:40-05:00pm  TR.01.13

06.01 Undergrad Research Symposium
Chair: Kathereine Kantardjieff
D1

01:30-02:00pm  06.01.1
Introduction. Kathereine Kantardjieff.

02:00-02:30pm  06.01.2

02:30-03:00pm  06.01.3

03:00-03:30pm Coffee break

03:30-04:00pm  06.01.4

04:00-04:30pm  06.01
A Model of the Alpha Domain Bound to DNA. Angelica Trammell, Doba Jackson, Chelley Lawson, Samuel Griffin, Ashlee Walters, Tiffany Dean.

Professional Odysseys
Chair: Jamaine Davis
Rhythms 1 (2nd floor)  1:30pm

Career Panel
Lorena S. Beese, James B. Duke Professor of Biochemistry, Duke University

Andy Howe, President and CEO at Emerald BioStructures and BioSystems, Co-Principal Investigator at Seattle Structural Genomics Center for Infectious Disease

Christopher Incarvito, Director, chemical and biophysical instrument center, Yale University
08.06 Microcrystals and Back to Merging Datasets
Chairs: Dominika Borek & Alex Soares Borgne

01:30-02:00pm  08.06.1
The Pervasive Problem of Crystal Non-Iso-
morphism. Zbyszek Otwinowski, Dominika
Borek, Johan Hattne, Marcin Cymborowski,
Wladek Minor.

02:00-02:30pm  08.06.2
Multi-Crystal Data Reduction at Diamond
Light Source. Graeme Winter.

02:30-03:00pm  08.06.3
Multi-Crystal Anomalous Diffraction for Mac-
romolecular Phasing. Qun Liu, Zhen Zhang,
Zahra Assur, Filippo Marcia, Wayne Hendrick-
son.

03:00-03:30pm  08.06.4
Coffee Break

03:30-04:00pm  08.06.4
Data Collection and Processing From Micro-
crystals of the Beta2-Adrenergic Receptor.
Bill Weis.

04:00-04:30pm  08.06.5
Systematically Study of Frozen Crystals Non-
Isomorphism: Example Case of Insulin Cryst-
tals. Rita Giordano, Sean McSweeney, Alex-
ander Popov.

04:30-05:00pm  08.06.6
Automated Acoustic Methods for Crystal-
lization, Crystal Improvement, and Crystal
Mounting. Alexei Soares, Allen Orville, Krystal
Cole, Joseph Olechno, Richard Ellson, John
 Skinner, Robert Sweet, Annie Heroux, Mat-
thew Engel, Marc Allaire.

2011 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. Selec-
tions 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 ........................................ Rebekah Nash, Univ. North Carolina, Chapel Hill .................08.09.6
General Interest .......................... Jason Mercer, Memorial Univ. of Newfoundland .......................02.01.3
Materials Science .................... Phoebe Allan, Univ. of St. Andrews, UK .....................08.08.1
Powder Diffraction ..................... Kevin Rhodes, Univ. of Tennessee, Oak Ridge .......... 08.07.10
Small Molecules .......................... John Sander, Univ. of Iowa, Iowa City .................05.02.13
Small Angle Scattering ............ Thomas Grant, Hauptman-Woodward Inst, Buffalo NY ......04.03.5
Synchrotron Radiation............... Lauren Hatcher, Univ. of Bath, UK .....................TR.01/05.01.4
Young Scientist .......................... Karen Ruane, McGill Univ., Montreal Canada ........... SP01.2
**TUESDAY, MAY 31**

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<td>07:30am</td>
<td>Speaker Ready Room</td>
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<td>07:30am</td>
<td>Council Meeting Room</td>
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<td>10:00am</td>
<td>Exhibit Show</td>
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<td>10:00am</td>
<td>Service &amp; Small Molecules Joint SIG Meeting</td>
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<td>12:00pm</td>
<td>Young Scientist SIG Meeting</td>
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<td>05:00pm</td>
<td><strong>All Member Business Meeting</strong></td>
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<td>05:30pm</td>
<td>Napoleon Ballroom</td>
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<td>10:50-11:10am</td>
<td>The Structural Basis of Assembly Stimulated GTP Hydrolysis by Human Dynamin. Fred Dyda,</td>
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<td>Joshua S. Chappie, Sharmistha Acharya, Marilyn Leonard, Sandra L. Schmid.</td>
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<td>10:50-11:10am</td>
<td>Structure of the DNA Glycosylase Alka in Complex With Undamaged DNA. Brian Bowman,</td>
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<td>Seongmin Lee, Shuyu Wang, Gregory Verdine.</td>
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<td>11:10-11:30am</td>
<td>The Crystal Structure of the Intron Debranching Enzyme in Complex With a Substrate</td>
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<td>Analog Provides Insights Into Substrate Recognition and Raises Questions Regarding Which</td>
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<td>Metal Cofactors Are Bound in the Enzyme Active Site. Eric Montemayor, Jonathan</td>
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<td>Schuermann, Alexander Taylor, Scott Stevens, John Hart.</td>
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<td>11:30-11:50am</td>
<td>Neutron Crystal Structures of Human Carbonic Anhydrase II at Different Ph Reveal</td>
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<td>Implications for Catalysis. Zoe Fisher, Andrey Kovalevsky, Marat Mustyakimov, John</td>
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<td>Domsic, Robert McKenna, David Silverman, Paul Langan.</td>
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<td>11:50-12:00pm</td>
<td>Molecular Basis of 1,6-Anhydro Bond Cleavage and Phosphoryl Transfer by</td>
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<td>Pseudomonas Aeruginosa 1,6-Anhydro-N-Acetylmuramic Acid Kinase. John-Paul Bacik,</td>
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<td>Garrett Whitworth, KeithStubbs, Anuj Yadav, Dylan Martin, Ben</td>
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<td>Bailey-Elkin, David Vocadlo, BrianMark.</td>
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<td>01.03.5</td>
<td>Structure of the DNA Glycosylase Alka in Complex With Undamaged DNA. Brian Bowman,</td>
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<td>Seongmin Lee, Shuyu Wang, Gregory Verdine.</td>
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<td>01.03.8</td>
<td>The Crystal Structure of the Intron Debranching Enzyme in Complex With a Substrate</td>
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<td>Analog Provides Insights Into Substrate Recognition and Raises Questions Regarding Which</td>
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<td>Metal Cofactors Are Bound in the Enzyme Active Site. Eric Montemayor, Jonathan</td>
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<td>Schuermann, Alexander Taylor, Scott Stevens, John Hart.</td>
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<td>01.03.7</td>
<td>Neutron Crystal Structures of Human Carbonic Anhydrase II at Different Ph Reveal</td>
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<td>Implications for Catalysis. Zoe Fisher, Andrey Kovalevsky, Marat Mustyakimov, John</td>
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<td>Domsic, Robert McKenna, David Silverman, Paul Langan.</td>
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<td>01.03.6</td>
<td>Molecular Basis of 1,6-Anhydro Bond Cleavage and Phosphoryl Transfer by Pseudomonas</td>
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<td>Aeruginosa 1,6-Anhydro-N-Acetylmuramic Acid Kinase. John-Paul Bacik, Garrett Whitworth,</td>
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<td>KeithStubbs, Anuj Yadav, Dylan Martin, Ben Bailey-Elkin, David Vocadlo, BrianMark.</td>
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<td>01.03.4</td>
<td>Solid-State Structure Determination of Water-Soluble Iridium Half-Sandwich Complexes for</td>
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<td>Catalytic Water Oxidation. Nathan Schley, James Blakemore, Christopher Incarvito, Gary</td>
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<td>Brudvig, Robert Crabtree.</td>
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</tbody>
</table>

**SP.03 Warren Award to Keith Moffat**
Award presentation to Keith Moffat by President Thomas Koetzle.
D2-D3

**01.03 Structural Enzymology II - Mechanistic**
Chair: Zachary Wood Borgne

**01.03.1**
The Structural Basis of Assembly Stimulated GTP Hydrolysis by Human Dynamin. Fred Dyda, Joshua S. Chappie, Sharmistha Acharya, Marilyn Leonard, Sandra L. Schmid.

**01.03.2**
Characterization of HPXO, a Novel Fad-Dependent Urate Oxidase. Katherine Hicks, Sean O’Leary, Tadhg Begley, Steven Ealick.

**01.03.3**

**05.01 Cool Structures**
Chair: Allen Oliver Maurepas

**05.01.1**
9:15-09:30am 05.01.2

09:30-09:45am 05.01.3
Three Strikes and You’re Out? Patrick Carroll.

09:45-10:00am 05.01.4

10:00-10:30am Coffee break

10:30-10:45am 05.01.5

10:45-11:00am 05.01.6
Three Polymorphs Or how to Grow Crystals From a Melt. Ilia Guzei, Erica Gunn, Lara Spencer, Jennifer Schomaker, Jared Rigoli.

11:00-11:15am 05.01.7
Broad Neutralization of Influenza Virus and Implications for a Universal Flu Vaccine . Ian Wilson, Damian Ekiert, Gira Bhabha, Cyrrle Dreyfyl.

11:15-11:30am 05.01.8
Structure and Disorder in K4(NCS)6 'x(OCMe2). Saul Lapidus, Kevin H. Stone, Endrit Shurda, Joel S. Miller, Peter W. Stephens.

11:30-11:45am 05.01.9

11:45-12:00pm 05.01.10
Ordered Surface Waters Bind Antifreeze Proteins to Ice. Peter L. Davies, Robert L. Campbell, Christopher P. Garnham.

07.01 Fast Science
Chair: Tim Graber & Marco Cammarata
D2-D3

09:00-09:30am 07.01.1
Picosecond Pump-Probe X-Ray Liquidography (Solution Scattering) to Probe Solution-Phase Structural Dynamics. Hyotcherl Ihee.

09:30-10:00am 07.01.2

10:00-10:30am Coffee Break

10:30-11:00am 07.01.3

11:00-11:30am 07.01.4

11:30-12:00pm 07.01.5

08.08 The Devil is in the Details: Local Structure and Diffuse Scattering
Chair: Karena Chapman
D1

09:05-09:30am 08.08.1

09:30-09:45am 08.08.2
Unusual Effect of Pressure on the Coefficient

09:45-10:00am  08.08.3

10:00-10:30am Coffee Break

10:30-10:55am  08.08.4

10:55-11:10am  08.08.5
_In situ_ Pair Distribution Function (PDF) and X-Ray Diffraction (XRD) Studies of Conversion Reactions With Lithium in Bismuth Oxyfluorides. Olaf Borkiewicz, Olaf Borkiewicz, Karena Chapman, Lin-Shu Du, Andrew Gmitter, Glen Amatucci, Clare Grey, Peter Chupas.

11:10-11:35am  08.08.6

11:35-11:50am  08.08.7

11:50-12:00pm  08.08.8

07.02 Maximizing the Scientific Results of Your Synchrotron Visit
Chair: Stephan Ginell Maurepas

01:30-02:00pm  07.02.2

02:00-02:30pm  07.02.3

02:30-03:00pm  07.02.4

03:00-03:30pm Coffee Break

03:30-04:00pm  07.02.5
Isomorphous Replacement From Selenomethionine-Containing Proteins Using UV-Induced Radiation Damage. Daniele de Sanctis, Santosh Panjikar, Paul Tucker.

04:00-04:30pm  07.02.6

04:30-05:00pm  07.02.7
Evolving Crystallographic Tools and Techniques at GM/CA Cat That Target Challenging Samples. Craig Ogata, Ruslan Sanishvili, Mark Hilgart, Sergey Stepanov, Michael Becker, Venugopalan Nagarajan, Shenglan Xu, Oleg Makarov, Janet Smith, Robert Fischetti, Sudhir Pothiineni, Derek Yoder, Stephen Corcoran.
08.09 Structural Enzymology III - Biology  
Chair: Michael Murphy  
D2-D3

01:30-02:05pm  08.09.1
Alleviating Anticancer Drug Toxicity by Inhibiting a Bacterial Enzyme. Matthew Redinbo, Bret Wallace.

02:05-02:40pm  08.09.2

02:40-03:00pm  08.09.3
A Structural Model for Binding of the Serine-Rich Repeat Adhesin GspB to Host Carbohydrate Receptors. Tasia Pyburn, Barbara Bensing, Yan Xiong, Bruce Melancon, Thomas Tomsiaik, Victoria Yankovskaya, Gary Cecchini, Gary Sulikowski, Paul Sullam, Tina Iverson, Nicholas Ward, Kevin Oliver.

03:00-03:30pm Coffee Break

03:30-04:05pm  08.09.4
A Structural Paradigm for Host Cell Invasion by Apicomplexan Parasites. Martin Boulanger, Michelle Tonkin, Magali Roques, Maryse Lebrun.

04:05-04:30pm  08.09.5
Structural Insights Into Iron Pirating by Pathogenic neisseria. Nicholas Noinaj.

04:30-04:55pm  08.09.6

08.10 Educational Inspiration: Crystallographic Teaching Techniques  
Chair: Amy Sarjeant Borgne

01:25-01:50pm  08.10.1
What's All This MoOing About? David Watkin.

01:50-02:15pm  08.10.2
Visualizing Symmetry and Chemical Structure in the Undergraduate Curriculum. Dean Johnston.

02:15-02:35pm  08.10.3

02:35-03:00pm  08.10.4
Teaching Crystallography at MIT. Peter Mueller.

03:00-03:30pm Coffee Break

03:30-03:55pm  08.10.5

03:55-04:20pm  08.10.6

04:20-04:45pm  08.10.7
Crystallography Experiments for an Undergraduate Laboratory. Nigam Rath, Christopher Spilling, Stephen Holmes.

04:45-05:05pm  08.10.8
Making Movies of Solid-State Transformations: Professor Inspires Students and Students Inspire Professor. Bruce Foxman, Aaron R. Gell, Shai R. Posner.
08.11 Diffraction Studies of Industrial Materials  
Chairs: Yan Gao & Bryan Chakoumakis  
D1

01:30-02:00pm 08.11.1  

02:00-02:15pm 08.11.2  

02:15-02:45pm 08.11.3  

02:45-03:00pm 08.11.4  
Crystal Structure of Monoclinic Sr24 Ca06 Al2 O6. James Kaduk, Winnie Wong-Ng, Joseph Golab.

03:00-03:30pm  
Coffee Break

03:30-04:00pm 08.11.5  
Microelectronics Materials and Synchrotron X-Rays: Metal Silicide Research by IBM at the NSLS. Jean Jordan-Sweet, Christian Lavoie.

04:00-04:15pm 08.11.6  

04:15-04:45pm 08.11.7  

EVENING SESSIONS

06.02.2 Would You Publish This?  
Chair: Carla Slepodnick  
Borgne 07:00pm  
sponsored, in part, by Agilent Technologies, Crystallographic Resources, Inc., and Ellen Mathena

06.02.2  
Tethered Bis-Phenanthroline Copper Complexes: Dimers, Trimers, Polymers. Allen Oliver, Luis Lemus, Graham Lappin.

06.02.3  

06.02.4  

06.02.5  
What If We Cannot Balance the Charges? Khalil A. Abboud, Tu Nguyen, Constantinos Efthymiou, George Christou.

06.02.6  

06.02.7  
A Case of a Poorly Diffracting Crystal. Larry Falvello.

Panel Discussion: Industrial Access to National User Facilities  
Chair: Jim Kaduk  
D1 07:30pm  
Dean Myles (SNS/ORNL)  
Dennis Mills (APS/ANL)  
Jun Wang (NSLS/BNL)  
Michel Fodje (CLS)
SP.04 Fankuchen Award
Award presentation to David Watkin by President Thomas Koetzle.
D2-D3
08:00-08:50am SP.04.1

01.04 Membrane Protein Crystallization
Chair: Michael Wiener
Borgne

09:00-09:30am 01.04.1
High Throughput Production of Membrane Proteins for Crystallography. NYCOMPS, Brian Kloss, Renato Bruni, Marco Punta, Burkhard Rost, Arianne Morrison, Filippo Mancia, Larry Shapiro, Wayne Hendrickson.

09:30am-10:00am 01.04.2
Membrane Protein Pre-Crystallization Screening. Michael Wiener, James Vergis, Michael Purdy, Rachel Reuther.

10:00-10:30am Coffee break

10:30-10:45am 01.04.3
Expanding Crystallization Optimization Capacity Using Alchemist-tm DT. Jian Xu, Matthew Lundy, Michael Willis.

10:45-11:00am 01.04.4
A Fast and Fully Automated Solution for Lipidic Cubic Phase (LCP) Screening Using Mosquito LCP. Joby Jenkins, Patricia Edwards, Rob Lewis, Joanne Franklin.

11:00-11:30am 01.04.5
Structure-Function Studies of Family B Gp-crs and Their Signaling Complexes. Hilary Stevenson, Qiangmin Zhang, Filippo Pullara, Guillermo Calero.

11:30-12:00pm 01.04.6
Current Progress on Membrane Protein Femtosecond Nanocrystallography. Mark Hunter, John Spence, Henry Chapman, Rick Kirian, Tom White, Uwe Weierstall, Anton Barty, Dan DePonte, R. Bruce Doak, Petra Fromme.

04.03 Information in SAXS/WAXS Data
Chair: Hiro Tsuruta & Lee Makowski
Maurepas

09:00-09:30am 04.03.1
Structural Determinants of Multidomain Complexes: Integrating SAXS and Biophysical Computations. Sichun Yang.

09:30-10:00am 04.03.2
Robust, High-Throughput Solution Structural Analyses by Small Angle X-Ray Scattering (SAXS). Michal Hammel.

10:00-10:30am Coffee Break

10:30-11:00am 04.03.3

11:00-11:30am 04.03.4
Snapshot SAXS for ab initio Imaging From Spatial Correlations. Richard Kirian, Kevin Schmidt, Dilano Saldin, John Spence.
11:30-12:00pm 04.03.5
DNA Conformations in Mismatch Repair Seen in Solution by X-Ray Scattering From Gold Nanocrystals. Greg Hura, Shelley Clarke, Marc Mendillo, Christopher Putnam, Richard Kolodner, A. Paul Alivisatos, John Tainer.

05.02 Modern Aspects of Crystal Engineering I
Chair: Travis Holman D2-D3

09:00-09:30am 05.02.1

09:30-10:00am 05.02.2

10:00-10:30am Coffee Break

10:30-11:00am 05.02.3

11:00-11:20am 05.02.4

11:20-11:35am 05.02.5

11:35-11:50am 05.02.6
Guest-Free Cavatands: Low Packing Fraction Materials. Christopher Kane, K. Travis Holman.

11:50-12:00pm 05.02.7

12:00-01:30pm Lunch break

01:30-02:00pm 05.02.8

02:00-02:30pm 05.02.9

02:30-03:00pm 05.02.10

03:00-03:30pm Coffee Break

03:30-03:45pm 05.02.12

03:45-04:00pm 05.02.13

04:00-04:30pm 05.02.14

04:30-04:50pm 05.02.15
Crystal Engineering of Quaternary Ammonium Salts of a Morphinan Opioid Modulator: Impact of Hydration Behavior on Form Selection. Mark Oliveira, Magali Hickey, Mark Tawa, Julius Remenar, Carlos Sanrane, Cherie Guo, Kenneth Hardcastle, Bruce Foxman, Orn Almarsson.

04:50-05:10pm 05.02.16
WEDNESDAY, JUNE 1

08.13 Evolution of Powder Diffraction Software: In Honor of Lachlan Cranswick
Chair: Peter Stephens
D1

02:00-02:30pm 08.13.1
Discovery of Novel Fragment Inhibitors of Acetyl Coa Carboxyltransferase. Felix Vajdos, Marie Anderson, Kris Borzilleri, Venkataraman Thanabal.

02:30-03:00pm 08.13.2
Managing 2D and 3D Ligand Fragments From Disparate Large Resources for Structure Based Drug Discovery. Talapady Bhat.

08.13.3 03:00-03:30pm
Coffee Break

08.13.4 03:30-04:00pm
Structures of Human Hepatitis C Virus Ns5B Polymerase With Inhibitors Bound to the P495 and Primer Grip Sites Reveal Enzyme Flexibility. Steven Sheriff, Changhong Wan, Kevin Kish, Daniel Camac, Chong-Hwan Chang, Brett Beno, Xiaofan Zheng, Robert Gentles, Min Ding, Louis Chupak, Paul Morin, Mark Witmer, Thomas Hudyma, Feng He, Michael Poss, John Kadow, Karen Rigat, Ying-Kai Wang, Robert Fridell, Julie Lemm, Dike Qiu, Mengping Liu, Stacey Voss, Lenore Pelosi, Susan Roberts, Min Gao, Jay Knipe.

08.13.5 04:00-04:30pm

08.13.6 04:30-05:00pm

08.12 Macromolecular Assemblies
Chair: Chris Hill
Borgne

01:30-02:06pm 08.12.1
Structural Basis for Nucleosome Recognition by the RCC1 Chromatin Factor. Song Tan, Ravindra Makde, Joseph England, Jiehuan Huang, Hemant Yennawar.
02:06-02:24pm 08.12.2

02:24-02:42pm 08.12.3
Structural Insights Into Holoenzyme Assemblies and Substrate Preferences of Biotin-Dependent Carboxylases. Christine Huang, Liang Tong.

02:42-03:00pm 08.12.4
Structural Basis for Cooperative Recognition of RNA by NUSB and NUSE During Transcription Antitermination. Jason R. Stagno, Amanda S. Altieri, Mikhail Bubunenko, Sergey G. Tarasov, Jess Li, Donald L. Court, R. Andrew Byrd, Xinhua Ji.

03:00-03:30pm Coffee Break

03:30-04:06pm 08.12.5
Structure of the HIV Capsid. Owen Pornillos, Barbie Ganser-Pornillos, Mark Yeager.

04:06-04:24pm 08.12.6

04:24-05:00pm 08.12.7
Dynamic Structural Mechanisms Underlying Ubiquitin-Like Protein Conjugation. Brenda Schulman.

08.14 Diffraction Studies of Magnetic Materials
Chair: Clarina De La Cruz D1

01:55-02:20pm 08.14.1
Superconductivity in Iron Chalcogenides. Mark Green.

02:20-02:35pm 08.14.2

02:35-03:00pm 08.14.3

03:00-03:30pm Coffee Break

03:30-03:55pm 08.14.4
Geometrically Frustrated Magnetism - a New Route to Room Temperature Spintronics. Andrew Wills, Laura Fenner.

03:55-04:20pm 08.14.5

04:20-04:35pm 08.14.6
Phase Separation and Phase Transitions in Multiferroic K3Fe5F15. Sandra Reisinger, Philip Lightfoot, Marc Leblanc, Anne-Marie Mercier.

04:35-05:00pm 08.14.7

05:00-05:15pm 08.14.8
08.15 Data Processing with the Pros
Ed Collins & Andy Torelli
Borgne
sponsored, in part, by DECTRIS, Ltd., Rayonix and Rigaku

09:00-09:30am  08.15.1
Data Processing With XDS. Kay Diederichs.

09:30-10:00am  08.15.2
Mosflm & iMosflm. Harry Powell, Andrew Leslie.

10:00-10:30am Coffee Break

10:30-11:00am  08.15.3
Professional Results From Diffraction Images With D*Trek. James Pflugrath.

11:00-11:30am  08.15.4

11:30-12:00pm  08.15.5

08.16 Earth Materials
Chairs: John Parise & Ian Swainson
D1

09:00-09:20am  08.16.1

09:20-09:40am  08.16.2

09:40-10:00am  08.16.3

10:00-10:30am Coffee Break

10:30-10:45am  08.16.4
Mendeleevite-(Ce), a New Mineral and a Potential New Microporous Material. Elena Sokolova, Frank Hawthorne, Leonid Pautov, Atali Agakhanov, Vladimir Karpenko.

10:45-11:00am  08.16.5
Short-Range Constraints on Chemical and Structural Variations in Bavenite. Frank Hawthorne, Aaron Lussier.

11:00-11:15am  08.16.6
Braitschite: a Crystallographic Challenge and a Structure to Show for It. Clare Rowland, Christopher Cahill, Jeffrey Post.

11:15-11:30am  08.16.10
In-situ Study of Kerogen Release and Metamorphism in Oil Shale by SANS. Kenneth

11:30-11:45am 08.16.11 X-Ray Analysis of Ferrous and Manganese-Ferrous Ores From Lakes and Marshes of Vologda Region. Nikolay Fedorchuk, Anton Chuev, Anatoly Pichurin.

11:45-12:00pm 08.16.12 Hydrated Sodium-Magnesium Sulfate Minerals Associated With Inland Saline Systems. Evelyne Leduc, R.C. Peterson.

08.17 Combined Techniques for Determining the Structure of Complexes and RNAs in Solution
Chairs: Yun-Xing Wang & John Tainer Maurepas

09:00-09:25am 08.17.1 Accurate Conformations, Assemblies and Structures of Macromolecules in Solution by X-Ray Scattering (SAXS) Combined With Crystallography. John Tainer, Robert Rambo, Greg Hura, Michal Hammel.

09:30-09:55am 08.17.2 Solution Structure of the 128 kDa Enzyme I Dimer from Escherichia coli and its 146 kDa Complex With HPr Using Residual Dipolar Couplings and Small and Wide Angle X-Ray Scattering. Marius Clore, Yuki Takayama, Alexander Grishaev, Jeong-Yong Suh, Charles Schwieters.

10:00-10:25am 08.17.3 Combined Use of SAXS and NMR for Structural Determination of Large RNAs and RNA Complexes in Solution. Xiaobing Zuo, Jinbu Wang, Ping Yu, Yun-Xing Wang.


11:05-11:20am 08.17.5 Quantitative Assessments of Flexibility and Validation of Biopolymer Models Using the Porod-Debye Law. Robert Rambo, John Tainer.


11:45-12:00pm 08.17.7 Time-Resolved SAXS Studies Revealed Crucial Roles of Autoproteolysis in a T=4 Virus Maturation. Tsutomu Matsui, John Johnson, Hiro Tsuruta.

12:05-12:20pm 08.17.8 Elucidating the Substrate Interaction Mechanism of the Hsp90 Molecular Chaperone. Timothy Street, Laura Lavery, David Agard.

08.18 Small Molecule Molecular Machines
Chair: Christopher Incarvito
D2-D3
sponsored, in part, by Yale University

09:00-09:30am 08.18.1 Mechanical Properties in Supramolecular Assemblies. Jeremiah Gassensmith.

09:30-10:00am 08.18.2 Ultra-Fast Rotors for Molecular Machines and Functional Materials Via Halogen Bonding: Crystals of 1,4-Bis(lodoethynyl)Bicyclo[222] Octane With Distinct Gigahertz Rotation at Two Sites. Cortion Vogelsberg, Cyprien Lemouchi, Leokadiya Zorina, Sergey Simonov, Patrick Batalia, Stuart Brown, Miguel Garcia-Garibay.
### 02.02 General Interest-II

**Chair:** Allen Oliver  
**D1**

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<tr>
<td><strong>02:00-02:15pm</strong></td>
<td><strong>02.02.1</strong> Applications of Two-Dimensional X-Ray Diffraction on Single-Crystal CCD Instruments.</td>
<td>Charles Campana, Baoping Bob He, Brian Jones, Holger Cordes.</td>
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<td><strong>02:00-02:15pm</strong></td>
<td><strong>02.02.2</strong> High-Brilliant X-Ray Sources for Chemical and Biological Crystallography in the Home Lab: An Update.</td>
<td>Juergen Graf, Carsten Michaelsen, Matthew Benning.</td>
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<td><strong>02:00-02:15pm</strong></td>
<td><strong>02.02.3</strong> The WWPDB X-Ray Validation Task Force, Low-Resolution Model Accuracy, and Visualizing Clusters of Local Error.</td>
<td>Bradley Hintze, Christopher Williams, Jane Richardson, David Richardson.</td>
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<td><strong>02:15-02:30pm</strong></td>
<td><strong>02.02.4</strong> Data Quality in Area Detector Diffraction Experiments.</td>
<td>Mathias Meyer.</td>
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<td><strong>02:30-02:45pm</strong></td>
<td><strong>02.02.5</strong> Better Instrument Design for Better Data.</td>
<td>Michael Ruf, Gary Bryant, Joerg Kaercher, Detlef Bahr, Christoph Ollinger, Brian Michell.</td>
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**08.19 Phasing and Refinement for Dummies: No Book Required**  
**Chairs:** Ed Collins & Andy Torelli  
**Borgne**  
*Supported, in part, by Rigaku*

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<tr>
<td><strong>01:00-01:15pm</strong></td>
<td><strong>08.19.1</strong> Automated Processing With Added Value.</td>
<td>Clemens Vonrhein, Claus Flensburg, Peter Keller, Włodek Paciorek, Andrew Sharff, Oliver Smart, Thomas Womack, Gerard Bricogne.</td>
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<td><strong>02:15-03:00pm</strong></td>
<td><strong>08.19.2</strong> Picking the Low-Hanging Fruit With SHELXC/D/E.</td>
<td>George Sheldrick.</td>
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<td><strong>03:00-03:15pm</strong></td>
<td><strong>08.19.3</strong> Ribosomal Protein S19, a Rosetta Stone of Speciation.</td>
<td>William Duax, Robert Huether, David Dziak.</td>
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<td><strong>03:00-03:15pm</strong></td>
<td><strong>08.19.4</strong> Nucleation and Crystallization Kinetics in Powders Probed by Second Order Nonlinear Optical Imaging of Chiral Crystals (SONICC).</td>
<td>Garth Simpson.</td>
</tr>
</tbody>
</table>
03:30-04:15pm 08.19.3 Macromolecular Refinement Program - REFMAC. Garib Murshudov.

04:15-05:00pm 08.19.4 Crystallographic Structure Solution Using Phenix. Pavel Afonine.

08.21 New Bio-Science from Emerging Opportunities and Sources
Chair: Bob Sweet Maurepas

01:30-01:53pm 08.21.1 Femtosecond Nanocrystallography of Membrane Proteins. Petra Fromme.


02:15-02:38pm 08.21.3 In situ Coherent Diffraction Imaging of Cellulose Crystals. Lee Makowski, Jyotsana Lal, Ross Harder, Ian Robinson.

02:38-03:00pm 08.21.4 Neutron Structure of Type-III Antifreeze Protein Leads to a Model of AFP-ICE Interface. Alberto Podjarny, Howard Eduardo, Matthew Blakeley, Michael Haertlein, Isabelle Petit-Haertlein, Andre Mitschler, Stuart Fisher, Alexandre Cousido-Siah, Alexandre Popov, Tania Petrova.

03:00-03:30pm Coffee Break

03:30-03:53pm 08.21.5 Combining Joint X-Ray/Neutron Crystallography and Quantum Enzymology (Quene) to Study Enzyme Mechanisms. Andrey Kovalevsky, Matt Challacombe, Nicolas Bock, Zoe Fisher, Marat Mustyakimov, Paul Langan.


04:15-04:38pm 08.21.7 Long-Wavelength Macromolecular Crystallography - Challenges and Opportunities. Armin Wagner.

04:38-05:00pm 08.21.8 Next Generation X-Ray and Neutron Macromolecular Refinement Using a Polarizable Force Field. Timothy Fenn, M.J. Schnieders, M. Mustyakimov, C. Wu, P. Langan, V.S. Pande, A.T. Brunger.

TR.01/05.01 Transactions continued & More Cool Structures
Morning Chair: Jason Benedict D2D-3

01:30-01:50pm TR.01/05.01.1 On the Use of Calculated Ads for Charge-Density Analysis of Normal-Resolution Data. Birger Dittrich.

01:50-02:10pm TR.01/05.01.2 Thermal Motion in Charge Density Studies Revisited. Alan Pinkerton, Vladimir Zhurov, Elizabeth Zhurova.

02:10-02:30pm TR.01/05.01.3 Determination of Time-Resolved Structural Changes of Dissolved Molecules With Xfel Radiation. Dilano Saldin, Hin-Cheuck Poon, Marius Schmidt, John Spence.

02:30-02:45pm TR.01/05.01.4 Thermal and Photocrystallographic Studies on a Nickel-Nitro Complex. Lauren Hatcher, Mark Warren, Paul Raithby.

02:45-03:00pm TR.01/05.01.5 Use of Imagine for Charge Density Studies. Parthapratim Munshi, Flora Meilleur, Tibor Koritsanszky, Robert Blessing, Bryan Chakoumakos, Dean Myles.
03:00-03:30pm Coffee break

Afternoon Chair: Jeanette Karuse

03:30-03:45 TR.01/05.01.6
The Day I Broke SHELX, and Other Synchrotron Anecdotes. Christine Beavers, Spyros Perlepis, Simon Teat, Marilyn Olmstead, Patrick Gamez.

03:45-04:00pm TR.01/05.01.7

04:00-04:15pm TR.01/05.01.8
Crystal Structure of New Superconducting Materials MxFe2-x/2Se2: Twinning vs. Disorder. Peter Zavalij, Mark Green.

04:15-04:30pm TR.01/05.01.9
Addressing Data Collection and Structure Solution Challenges From Light-Atom Clathrates With Very Large Z'. Jesse Rowsell, Matthias Zeller, Charles Campana.

04:30-04:45pm TR.01/05.01.10
Three New Endohedral Fullerenes, Sm2@C88, Sm2@C90, and Sm2@C92. Marilyn Olmstead, Brandon Mercado, Christine Beavers, Alan Balch, Hua Yang, Ziyang Liu.

04:45-05:00pm TR.01/05.011
(1,2,3-Trimethylpyridinium) 2Cu5Cl10-Linear Pentacopper(II) Complexes Crosshatched to Form an Egg-Tray Template. Marcus Bond.
**POSTER PRIZES**

**Pauling Poster Prize, Canadian and IUCr Poster Prize**
The Pauling Poster Prize was established by the ACA, and is supported by member contributions, to honor Linus Pauling. Pauling was one of the pioneers in American structural research and was very supportive of the ACA. At each annual meeting, the five best graduate or undergraduate poster presentations receive Pauling awards. Each award consists of $200, a complimentary banquet ticket, and a copy of a Linus Pauling book. An additional Pauling Prize sponsored by the Canadian Division of the ACA and the Canadian National Committee of the IUCr, will be given to the highest ranked graduate or undergraduate poster from a Canadian laboratory. Honorable mention awards for this prize are also made; they consist of a complimentary banquet ticket. IUCr Poster Prize: The IUCr Executive Committee is pleased to continue a series of IUCr awards presented at meetings of the regional affiliates and national crystallographic associations. The award is complimentary online access to all IUCr journals for one year or a complimentary volume of International Tables or other IUCr publication.

**Journal of Chemical Crystallography Prize**
The best student poster presentation in the area of chemical crystallography or small molecule structure determination and analysis is sponsored by Springer's Journal of Chemical Crystallography (<www.springer.com>). The winner will receive their personal choice of books from Springer’s extensive portfolio of titles.

**RCSB Protein Data Bank Poster Prize**
This 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 RCSB PDB website and newsletter. For more information, see www.rcsb.org/pdb

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

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

**American Chemical Society's International Year of Chemistry Poster Prize**
The ACA is happy to announce a special poster prize for 2011- The American Chemical Society’s International Year of Chemistry Poster Prize. The award (an IPOD-Nano) is intended to recognize an outstanding poster contribution from a junior scientist (undergrad, grad or post-doc) in the area of Chemical Crystallography, or who has used crystallography to solve a chemical problem. The ACA gratefully acknowledges the American Chemical Society (www.acs.org/international) for this opportunity.
POSTER HANGING INSTRUCTIONS

Posters beginning with 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 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 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 from 5:30 - 7:30pm on the day to which you are assigned and remove your poster at the end of the session.

Sunday Posters

S01
Growing Lysozyme Crystals for Neutron Diffraction Beamlines. Elena Magay, Yoon Tae-Sung.

S03

S04

S05
Synthesis and Crystal Structure of the Double Perovskites Alabsbo6, With a = Ba2+ and Pb2+ and B = Mn2+, Co2+, Ni2+, Cu2+ and Zn2+. Diego Franco, Cecilia Blanco, Raul Carbonio.

S06
The Role of Ing4 and Ing5 Tumor Suppressors in Chromatin Remodeling and Disease. Karen Glass, Nehme Saksouk, Pedro Pena, Kyle Johnson, Tiffany Hung, Xiang-Jiao Yang, Jacques Cote, Or Gozani, Tatiana Kutateladze.

S08

S09
Joint X-Ray and Neutron Crystallography at the Protein Crystallography Station. Zoe Fisher, Andrey Kovalevsky, Marc Michael Blum, Marat Mustyakimov, Mary Jo Waltman, Paul Langan.

S10
Metal-Organometallic Frameworks. K. Travis Holman, Sayon A. Kumalah Robinson.

S11
Structural Determinants of Tobacco Vein Mottling Virus Protease Substrate Specificity. David Waugh, Ping Sun, Brian Austin, Jozsef Tozser.

S12
Structural Basis for Promoter -10 Element Recognition by the Bacterial RNA Polymerase Sigma-Subunit. Andrey Feklistov, Seth Darst.

S13

S14
Posters-S

S15

S16

S17
Hints for Refining Low-Resolution Protein X-Ray Structures. Vishal Koparde, Glen Kellogg, Neil Scarsdale.

S18
Alkali Metal-Coordination Cages for Selective Sulfate Binding and Separation. Arbin Rajbanshi, Arbin Rajbanshi, Bruce A. Moyer, Radu Custelcean.

S19
Structural Basis for 5'-Nucleotide Base-Specific Recognition of Guide RNA by Human AGO2. Filipp Frank.

S20
Wanted Defects and Distortions!. Melissa Menard, Gregory T. McCandless, Kandace R. Thomas, Julia Y. Chan.

S21

S22
SCrALS: Challenging Samples, Straightforward Solution - the Continuing Story. Allen Oliver, Jeanette Krause.

S23

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S28
Crystal Engineering the Covalent Bond. Leonard MacGillivray.

S29
Structural Characterization of An Unusual Heme Cofactor in Hydroxylamine Oxidoreductase. Peder Cedervall, Alan Hooper, Carrie Wilmot.

S30

S31
Non Ambient Crystallographic Studies of Dithienylethene Optical Molecular Switches. Christopher Woodall, Paul Raithby, David Allan.

S34
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S41
Insights Into Phenyl Motion During the Racemization of Mandelate by Mandelate Racemase. Adam Lietzan, Elise Pellmann, Mitesh Nagar, Jennifer Bourque, Stephen Bearne, Martin St Maurice.

S42

S43
Molecular Bases of Enantioselectivity of Haloalkane Dehalogenase DjbA. Yukari Sato, Zbynek Prokop, Jan Brezovsky, Ryo Natsume, Yuji Nagata, Jiri Damborsky, Toshiya Senda, Radka Chaloupkova.

S44
Comparison of the Molecular Structures of μ-oxo Iron(III) Porphyrin Malaria Pigment Model Compounds. Saifon Kohnhorst, Kenneth Haller.

S45
Water Dimers in the Structure of NiV2O6 2H2O. Aungkana Chatkon, Kenneth Haller.

S47
Disorder in the Dihydrate of a Derivative of Acyclovir. Montha Meepripruk, Kenneth Haller.

S48

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S51

S53
S54 Dispositions of the Rod-Like Solvates Cs2 and I2 in the Nanotubular-Like Packing of C70 Structures. Faye Bowles, Marilyn Olmstead, Alan Balch.


S56 Montmorillonite Modification by Cationic Surfactants. Ana Bianchi, M Fernandez, M Pantanetti, Raul Vina, Iris Torriani, Rosa M. Sanchez, Graciela Punte.


S60 Mail-In Crystallography: Convenient Use of the Canadian Macromolecular Crystallography Facility. Shaunivan Labiuk, James Gorin, Kathryn Janzen, Michel Fodje, Pawel Grochulski.


S64 Data Processing and Assessment of Quality in Time-Resolved Laue Diffraction of Excited Species of the Organometallic Complex Rh2(M-Pnp)2(Pnp)2Bph4. Anna Makal, Jason Benedict, Jaroslav Kalinowski, Jesse Sokolow, Elzbieta Trzop, Phillip Coppens.

S66 Effect of Supramolecular Structure on Molecular Structure in a Titanium(III) Oxalate Dimer: Ti2((-C2O4)(C2O4)2(H2O)6 2H2O. Orrasa In-Noi, Kenneth J. Haller.


S67 Recent Bio-Science From the Center for Structural Molecular Biology at Oak Ridge. Volker Urban, William Heller, Kevin Weiss, Hugh O’Neill, Sai Venkatesh Pingali, Shuo Qian, Dean Myles.


S72 X8 Prospector: Using In-House Screening to Help Improve Productivity During Synchrotron Trips. Matthew Benning.


S76 Rapid Automated Processing of Data (RAPD) Software Package. Jonathan Schuermann, David Neau, Frank Murphy.

S77 Improvements in High Pressure Research Capabilities on Beamline 1222 at the Advanced Light Source. Jason Knight, Alastair MacDowell, Simon Clark, Howard Padmore, Selva Raju, Bin Chen, Jinyuan Yan, Lowell Miyagi, Jane Kanitpanyacharoen, Quentin Williams.

S78 Structure of CFA/I Fimbriae from Entorotoxi-genic Escherichia coli, the Bacteria that Cause Diarrhea. Rui Bao, Esther Bullitt, Stephen J Savarino, Di Xia.

S79 A Novel High-throughput Approach for Purification and Reconstitution of Large Multi-protein Complexes. Filippo Pullara, Monica Calero, Qiangmin Zhang, Hilary Stevenson, Guillermo Calero.
Monday Posters

M01

M02

M03

M04

M05

M06
Structures of Inhibitor and Substrate Complexes of Golgi alpha-Mannosidase II Reveal the Basis for Fragment-Based Anti-Cancer Compounds. David Rose, Douglas Kuntz, Niket Shah, B. Mario Pinto.

M07

M08

M09
Structural Features of the Unusual Thiolase Olea That Facilitate Long-Chain Hydrocarbon Biosynthesis. Brandon Goblirsch, Janice Frias, Larry Wackett, Caroline Wilmot.

M10

M11
Systematic Approach to Better Crystals. Qiang (James) Zhao, Qian(Frank)Wang, Tian-tang Dong, Xinjun Liu, Xiaoshu Hou, Yuanna Zhai, Yujun Han, Huili Hou, Michelle Xia, Maxwell Wang.

M12
New Approaches to Time-Resolved Structural Studies of Macromolecules. Briony Yorke, Arwen Pearson, Mike Webb, Robin Owen.

M13

M14
Structural Insights Into Pseudouridine 5’-Phosphate Glycosidase. Siyu Huang, Steven Ealick.

M15
Structure of the CMP Hydrolase, MilB, Re-
M16
Structurally Similar But Functionally Different Zu5 Repeats in Human Erythrocyte Ankyrin. Mai Yasunaga, Jonathan Ipsaro, Alfonso Mondragon.

M17
Developing the Laue Method for Multicrystal Structure Determination. Doletha Szebenyi, Donald Bilderback, Ulrich English, Qingqiu Huang, Chae Un Kim, Irina Kriksunov, Mark Pfeifer, Detlef Smilgies.

M18

M19
A Paradigm for Glycan Acquisition by the Human Distal Gut Bacteroidetes: the Starch Utilization System (Sus) of Bacteroides Theiotaomicron. Nicole Koropatkin, Elizabeth Cameron, Eric Martens, Thomas Smith, Christopher Smith, Julie Bitech, Jeffrey Gordon.

M20
Correlating Changes in Structure and Function of Bacteroides Theiotaomicron Tetx2 to Fitness During Adaptation to Minocycline. Katarzyna Walkiewicz, Milya Davlieva, Christine Sun, Matthew Pena, Kelsey Lau, Yousif Shamoo.

M21

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M24
Invariom Modeling of a Short Fragment of “DNA”. Kevin Proepper, Julian Holstein, Birger Dittrich.

M25

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M28
Structure of Human C8 Protein Provides Mechanistic Insight Into Membrane Pore Formation by Complement. Leslie Lovelace, Christopher L. Cooper, James M. Sodetz, Lukasz Lebioda.

M29
Structure Function Studies of Vaccinia Virus
Host-Range Protein C7L Reveal a Unique Beta Fold Structure. Brian Krumm, Yongchao Li, Xiangzhi Meng, Yan Xiang, Junpeng Deng.


M31 High-Resolution Structures Reveal Halide Ion Binding to Optogenetic Chloride Sensors Constructed by Protein Engineering Automation. Weina Wang, Joshua Grimley, Lorena Beese, Homme Hellinga.


M33 Diagnosing Secondary Structure Pathologies at Low Resolution. Christopher Williams, Jane Richardson, David Richardson.

M34 D-Periodic Molecular Structure of Type II Collagen in situ to its Native Tissue. Joseph Orgel, Olga Antipova.


M36 Interactions Between HypE and HypF Hydrogen Maturation Factors. Svetlana Petkun, Rong Shi, Yonge Li, Jean Francois Trempe, Abdalin Asinas, Christine Munger, Miroslaw Cygler.

M37 Substrate and Product Complexes of Wild Type and Mutant E. coli QueD. Sue Roberts, Reid McCarty, Vahe Bandarian.


M42 Structure and Mechanism of Processing Alpha-Glucosidase I. Megan Barker, David Rose.

M43 Total Scattering at the Lujan Center. Katharine Page, Anna Llobet, Joan Siewenie.


M46 Neutron Single Crystal Diffraction From Experiment Planning to Analysis. Christina Hoffmann, Xiaoping Wang, Matthew Frost.
Janik Zikovky, Dennis Mikkelsen, Ruth Mikkelsen, Arthur Schultz, Peter Peterson.

M47

M48
Development of a Dedicated Pair-Distribution-Function Beamline at the Advanced Photon Source: Scientific Drivers and Opportunities. Peter Chupas.

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M56
Quantum Mechanical DFT Analysis of Copper Dynamic Behavior in Doped Zinc and Cadmium-Histidine Crystals. Michael Colaneri, Kristin Kirschbaum, Jacqueline Vitali.

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M59
‘Rational’ Stochastic Crystallization Screen Design for High-Throughput Protein Crystallography. Jared Liu, Li-Wei Hung.

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M64 Pseudoracemic Crystallization of a Small Protein Containing Pentafluorophenylalanine in Its Hydrophobic Core. David Mortenson, Kenneth Satyshur, Katrina Forest, Samuel Gellman.


M68 We Present a PDF Analysis of Different Species Intercalated in Nanoporous Materials the First Study is for a Series of Thiol-Functionalized Mesoporous Silicas With Different Mercaptopyropyl Content and Hg Loading, Materials That Are Effective Trapping Age. Mouath Shatnawi, Simon Billinge, Thomas Pinnavaia, Jame Dye, Emily McKimmy, Gianluca Paglia.

M69 Crystallization and Preliminary X-Ray Analysis of the Transcription Factor Complex of NKX25 and TBX5 With Target DNA. Lagnajeeet Pradhan, Sunil Kumar Gopal, Sandhya Ramesh, Hyun-Joo Nam Nam.


M72 Recent Developments in the SuperNova Dual Source Micro-focus Diffractometer. Zoltan Gal, Alexandra Griffin, Oliver Presly.

M73 Guided Ligand Replacement (GLR). Herbert Klei, Matt Pokross, Shana Posy, Thomas Terwilliger, Paul Adams, Nigel Moriarty.

M74 Crystal Structures of PKG ICE (92-227) with cGMP and cAMP Reveal the Molecular Details of Cyclic-nucleotide Binding. Gilbert Huang, Jeong Joo Kim, Darren Casteel, Taek Hun Kwon, Ronnie Ren, Peter Zwart, Jeffrey Headd, Nicholas Brown, Dar-Chone Chow, Choe Kim.

M75 Crystal Structure Analysis of Nectin and Nectin Like Molecule Family. Mamoru Suzuki, Hirotaka Narita, Atsushi Nakagawa.
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WAXS Studies of the Structural Diversity of Protein Ensembles. Lee Makowski.

T04
Macrosnap: Software for Rapidly Comparing, Clustering and Visualizing 3-D Protein Structures Mined From the PDB. Chris Gilmore, Stuart Mackay, Gordon Barr, Wei Dong, Adrian Lapthorn.

T05
Protein Structure Determination by Exhaustive Search of the RCSB Protein Data Bank Derived Databases. Ian Stokes-Rees, Piotr Sliz.

T06

T07
Identification of the DNA Repair Active Site of Topoisomerase V by Structural and Functional Studies. Rakhi Rajan, Rajendra Rajendra Prasad, Bhupesh Taneja, Samuel H Wilson, Alfonso Mondragon.

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Structural Studies on Therapeutic Antibodies for Prion Diseases. Michael James, Pravas Baral, Mridula Swayampakula, Barbara Wieland, Rahman Muhammad, M. Polymenidou, Adriano Aguzzi, Nat Kav.

T11
Ancestral Protein Sheds Light on Steroid Receptor Cross-Pharmacology. Eric Ortlund, Jeffrey Kohn.

T12
Structural, Computational, and Biophysical Studies of Monocarbam-Siderophore Conjugate, Mc-1. Seungil Han, Richard Zaniewski, Eric Marr, Brian Lacey, Andrew Tomaras, Arterm Evdokimov, J. Richard Miller, Xidong Feng, Kieran Geoghegan, Veerabahu Shanmugasundaram.

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The UvrA UvrB DNA Damage Sensor: Structure and Mechanism. David Jeruzalmi, Danaya Pakotiprapha, Martin Samuels, Koning Shen, Johnny Hu.

T15
Using a Conformationally-Dependent Stereoochemical Library Improves Crystallographic Refinement of Proteins. Dale Tronrud, Donald Berkholz, P. Andrew Karplus.
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MoleCoolQt - a Molecule Viewer for Charge-Density Research. Christian Huebschle, Birger Dittrich.

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Hydrogen Bonding in the Crystal Structures of Hydantoins and Related Molecules. Carl H. Schwalbe, Aurora J. Cruz-Cabeza.

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Hydroxyl Orientations in Celllobiose and Other Polyhydroxy Compounds - Modeling Vs Experiment. Alfred French, Gabor Csonka.

T28
Macromolecular Data Collection and Processing Using Crystalspro and the Supernova. Tadeusz Skarzynski.

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The HB2A High Resolution Powder Diffractometer at the High Flux Isotope Reactor. Clarina de la Cruz.

T35
Biophysical Analysis of Conformational Changes in Adeno-Associated Viruses Under Endosomal pH Conditions. Balasubramanian Venkatakrishnan, Shuo Qian, Barry Byrne, Nicholas Muzychka, Mavis Agbandje-McKenna, Robert McKenna.

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Removing a Persistent, Publication-Preventing Difference Peak From a Single-Crystal Structure Analysis. Larry Falvello, Sonia Martinez-Salvador, Babil Menjon.

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Unfurling of the F2 Ferm Domain of Merlin Tumor Suppressor. Sollepura Yogesha, Andrew Sharff, Marco Giovannini, Gerard Bricogne, Tina Izard.

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A Laboratory Information Management System for Macromolecular Crystallography Experiments at the Canadian Light Source. Kathryn Janzen, Michel Fodje, Pawel Grochulski, Shaunivan Labiuk, James Gorin.

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Crystal Structures of a Therapeutic Single Chain Antibody in Complex With Two Drugs of Abuse and Their Psychologically-Active Metabolites. Reha Celikel, Eric Peterson, Michael Owens, Kottayil Varughese.

T46
Improvements to On-Axis Visualization (OAV) at GM/CA CAT Beamlines at the APS. Nagarajan Venugopalan, Shenglan Xu, Steve Corcoran, Sudhir Pothineni, Oleg Makarov, Sergey Stepanov, Janet Smith, Robert Fischetti.
T47
Chemical Crystallography for Undergraduate Research: Unexpected and Fruitful Results. Gary Nichol, Stephanie Hurst, Edward Rajaseelan.

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A Salvage Protein Purification Approach in Mcsg High-Throughput Pipeline. Ruiying Wu, Hui Li, Gyorgy Babnigg, Youngchang Kim, Andrzej Joachimiak.

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C-Hal...Hal Nonbonded Intermolecular Interactions in Molecular Crystals. Raymond Davis.

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Cooling Rate- and Temperature-Dependence of a Highly Mobile “Flap” Covering the Active Site of Urease. Robert Thorne, Matthew Warkentin, Andrew Karplus.

T55
SONICC Miniaturization for Direct Implementation Onto Synchrotron Beamlines for Protein Crystal Detection and Automated Centering. Jeremy Madden, David Kissick, Garth Simpson.

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A Novel Approach to Automatic Scoring of Protein Drop Images Using UV Fluorescence. Max Petersen, Mandel Mickley, Chris Boarman, Giles Mullen.

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Three-Dimensional Models for All Binary and Ternary Protein Complexes of the Cyanobacterial Kaiabc Circadian Oscillator and the Clock Output Kinase Sasa. Rekha Pattanayek, Dwight Williams, Tetsuya Mori, Gian Rossi, Steven Weigand, Carl Johnson, Phoebe Stewart, Martin Egli.

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A High-Performance Small Angle X-Ray Scat-

T64
An Instrument for Fluorescence-Based Imaging and Scoring of Protein Crystallization Plates. Marc Pusey, Madhav Sigdel, Ramazan Aygeu.

T65
Structural Characterization of the Role of Nep1, a Psuedouridine N1-Specific Methyltransferase, in Ribosome Biogenesis. Nicole LaRonde-LeBlanc, Seth Thomas, Christopher Keller, Agnieszka Syzk, Joseph Cannon.

T66
Applications of Pairwise Comparison and Classification of the Ligand Binding Sites in Protein Three-Dimensional Structures. Stephane Richard, Moriaud Fabrice, Olivia Doppelt-Azeroual, Stephane Richard, Francois Delfaud.

T67
What We Know and Do Not Know From Several Structures of the Tautomerase Superfamily. Marvin Hackert, Guo Youzhong, Jeffrey Almrud, William Johnson Jr., Christian Whitman.

T68
XLF Regulates Filament Architecture of the XRCC4-Ligase IV Complex. Michal Hammel, Yaping Yu, Shujuan Fang, Susan Lees-Miller, John Tainer.

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Remote Access at LS-CAT. David Smith, Keith Brister, Max Brister.

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Crystal Structure of ER-resident Protein Disulfide Reductase ERdj5. Mamoru Suzuki, Masatoshi Hagiwara, Kenichi Maegawa, Jun Hoseki, Kazuhiro Nagata, Kenji Inaba.

T73
Crystal Structure of ER-resident Protein Disulfide Reductase ERdj5. Mamoru Suzuki, Masatoshi Hagiwara, Kenichi Maegawa, Jun Hoseki, Kazuhiro Nagata, Kenji Inaba.

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