

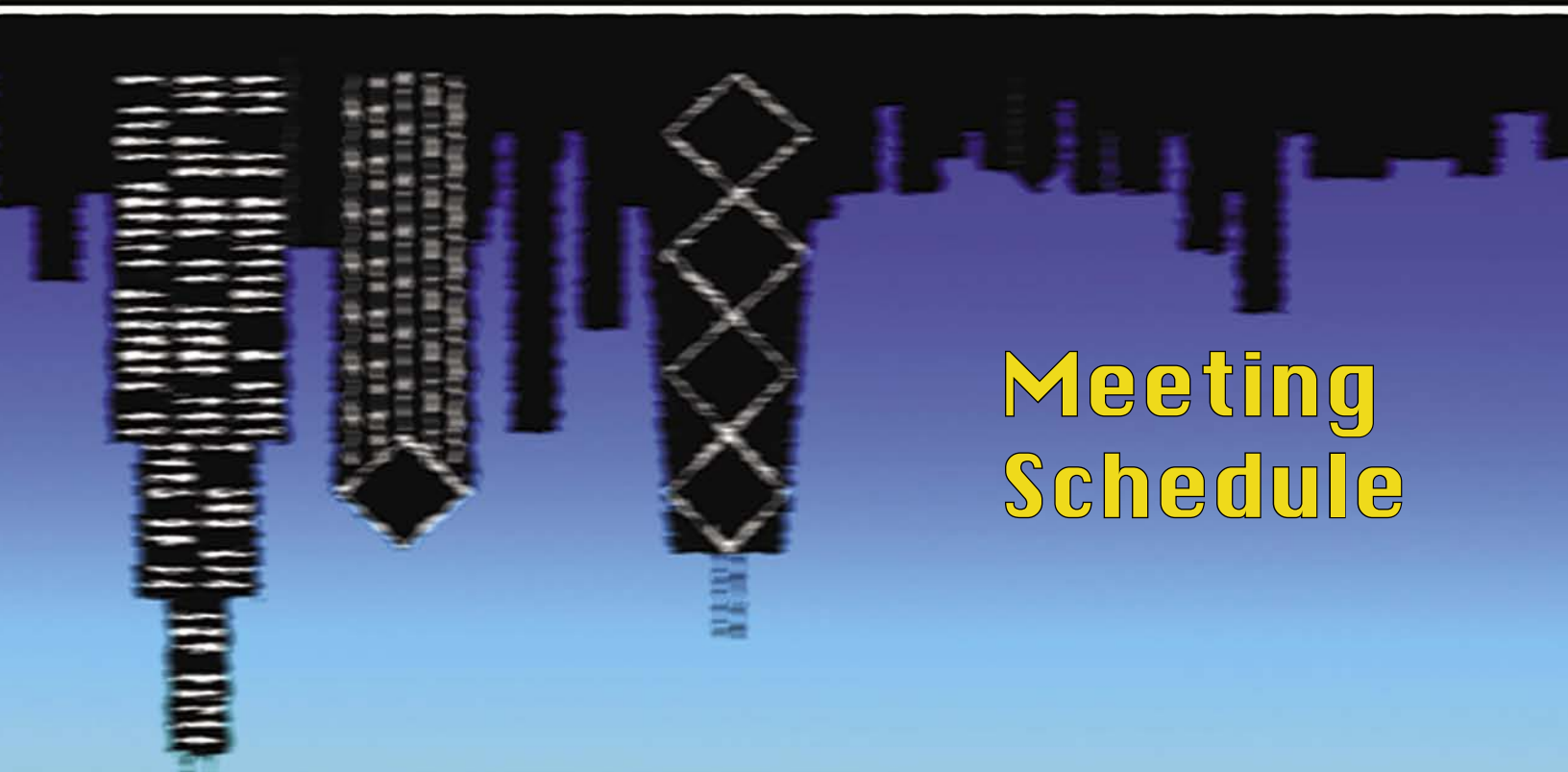
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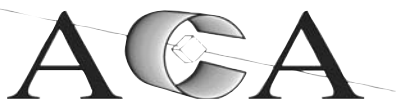
# ACA

# 2004

**American Crystallographic Association**

**Meeting  
Schedule**





# 2004 Annual Meeting

July 17 - 22

Chicago, Illinois

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## Program Committee Chairs

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## Program Committee

Lesa Beamer      Vivien Yee  
Alicia Beatty      Alexandre Yokochi  
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**ACA Registration Desk**

**07:30am-08:00pm**

**Opening Reception and Exhibit Show**

**08:00pm - nametag required for entry**

**Riverside Center East**

## THE FOLLOWING WORKSHOPS WILL BE HELD AT THE ADVANCED PHOTON SOURCE AT ARGONNE NATIONAL LAB

Registration for the following workshops is now closed. Pre-paid participants should pick up their conference packet at the ACA Registration Desk on Friday, July 16, 6:00pm-9:00pm inside the Hyatt. Buses will leave the Hyatt at 07:15a.m. on Saturday morning. Please be on time; if you miss the bus, additional transportation will not be available.

### WK.01 Hands On Workshop – MAD/SAD Phasing, Data Collection, Processing, and Structure Solution

Organizer: Jim Fait.

This all-day workshop will be structured as two half-day sessions, with the workshop participants split in two groups. One session will be at one of several APS beamlines, and will cover all aspects of collection of MAD and SAD data, including collection of diffraction data. The second session will cover the computing aspects of data reduction with various packages, scaling, evaluating quality of data, and structure solution and phase extension. Both practical examples and real data will be emphasized.

### WK.02 Small Molecule Crystallography at ChemMatCARS

Organizers: P. James Viccaro, Victor G. Young, Jr.

This all-day workshop will take place at the Advanced Photon Source at Argonne National Laboratory. It is intended particularly for small-molecule crystallographers and chemical crystallographers who have not yet conducted experiments at a synchrotron.

### WK.04 GM/CA - Synchrotrons for the Biologist

Organizers: Janet Smith, Ward Smith.

This workshop is intended as a primer on synchrotron structural biology, and will describe a new facility at the Advanced Photon Source (APS) at Argonne National Laboratory, established as a national user resource for biology by the National Institute of General Medical Sciences (GM) and the National Cancer Institute (CA), two institutes in the National Institutes of Health. Talks will describe how the special properties of synchrotron radiation are used for macromolecular crystallography, and the design and capabilities of the three GM/CA beamlines. This one-day workshop will focus on information for non-specialists and scientists interested in learning more about synchrotron structural biology and the new GM/CA facility in particular, including a tour of the GM/CA facilities at the APS.

### WK.05 APS/IPNS Tour

Organizer: Phillip Fanwick.

All-day tour of the synchrotron (APS) and neutron source (IPNS). The visit will include a tour of the two facilities and lectures illustrating the type of experiments run there. Practical details such as how to obtain beam time will be covered.

## WK03: A Protein Crystallographic Toolbox: CCP4 Software Suite and PDB Deposition Tools

**Columbus A-B**

Maeri Howard-Eales, Peter Briggs,  
Judith Flippen-Anderson, John Westbrook

### Morning session:

- 08:30 Introduction and Welcome
- 08:35 Introduction to CCP4 and the PDB. Maeri Howard-Eales and Judith Flippen-Anderson.
- 08:50 The CCP4 Package: General Overview. Peter Briggs.
- 09:20 Overview of Using CCP4 for PX. Martin Noble.
- 10:20 Coffee Break.
- 10:40 CCP4: Utilities, Tricks and Tips. Peter Briggs.
- 11:00 PDB\_EXTRACT and CCP4 - Making Deposition Easier. Shuchismita Dutta.
- 12:00 Lunch (provided onsite with ticket)

### Afternoon session:

- 12:45 Data Collection & Data Reduction Using MOS FLM and SCALA. Gwyndaf Evans.
- 01:45 Refinement Using REFMAC5. Roberto Steiner.
- 02:45 Coffee Break.
- 03:05 CCP4 Molecular Graphics: What Can It Do For You? Stuart McNicholas.
- 03:35 Data Deposition and Validation Using RCSB PDB Tools. Kyle Burkhardt.
- 04:35 Question and Answer.



# Sunday, July 18

Council Meeting Room	07:30am	Grand Suite 5	Fiber Diffraction SIG Meeting	05:15pm	Columbus C-D
Speaker Ready Room	07:30am	Columbus H	Powder Diffraction SIG Meeting	05:15pm	Columbus E-F
Interview Room	07:30am	Columbus G	Poster Session I	05:30pm	Riverside Center East
Exhibit Show	10:00am	Riverside Center East	MAR USA Evening Event	07:00pm	Blue Chicago Nightclub
IUCr Journals Commission	12:00pm	Grand Suite 3	Bruker AXS Dinner	07:30pm	(by invitation only)
Rigaku/MSC Luncheon	12:00pm	Crystal Ballroom	YSSIG Mentor/Mentee Dinner	07:30pm	Blue Agave Restaurant
PepcDB Working Group	02:00pm	Columbus G	<i>Thanks to Hampton Research, Nextal and Fluidigm for partial support of the Dinner</i>		
Small Molecules SIG Meeting	05:15pm	Columbus I-L			

## Opening Ceremony and Welcome

Columbus I-L

08:00-08:30am

Frances Jurnak, ACA President, Presiding

### 01.01 Structural Insights into Transcription

Columbus I-L Cynthia Wolberger, Presiding

08:30-09:00 01.01.01  
Structural Studies of Prokaryotic Transcription. Seth Darst.

09:00-09:30 01.01.02  
Structural Basis of Eukaryotic Transcription: Nucleotide Addition and the Role of TFIIB in Initiation. David Bushnell, Ken Westover, Ralph Davis, Roger Kornberg.

09:30-10:00 01.01.03  
Structural Mechanism of Carbon Catabolite Repression. Richard Brennan.

10:00-10:30 Coffee Break.

10:30-11:00 01.01.04  
Effector Binding to the LysR-Type Transcriptional Regulators, BenM and CatM. Cory Momany, Sandra Haddad, Todd Clark, Obidimma Ezezika, Ellen Neidle.

11:00-11:30 01.01.05  
Structural Analysis of Histone Methyltransferases. Rui-Ming Xu, Jinrong Min.

11:30-12:00 01.01.06  
Mechanism of NAD<sup>+</sup>-dependent Deacetylation by Sir2 Enzymes. Cynthia Wolberger, Jef Boeke, José Avalos.

### 01.02 Structural Analysis by Hybrid Methods

Columbus I-L Jamie Williamson, David Belnap, Presiding

01:30-02:00 01.02.01  
Structure and Function of Icosahedral Pyruvate Dehydrogenase Complexes from *B. stearothermophilus*. J.L.S. Milne, M.J. Borgnia, J. Lengyel, D. Shi, P. Zhang, R.N. Perham, S. Subramaniam.

02:00-02:30 01.02.02  
Joint X-ray and NMR Refinement of the L30e-mRNA Complex. James R. Williamson, Jeffrey A. Chao.

02:30-02:50 01.02.03  
Sleeping with the Enemy: Using Crystallography and NMR to Structurally Analyze the Redox Cycle of a Thiol-Disulfide Oxidoreductase. Christopher L. Colbert, Paul J. A. Erbel, Kevin Gardner, Johann Deisenhofer.

02:50-03:10 01.02.04  
Assessing Flexibility in the Multi-domain Filament Titin. Marco Marino, Laurent Kreplak, Mohamed Chami, Dimitri Svergun, Siegfried Labeit, Olga Mayans.

03:10-03:30 Coffee Break.

03:30-03:50 01.02.05  
Combining Raman Spectroscopy and Protein Crystallography to Analyse Reaction Intermediates in  $\beta$ -Lactamase Crystals. Pius Padayatti, Marion Helfand, Monica Totir, Marianne Carey, Andrea Hujer, Robert Bonomo, Paul Carey, Focco Van Den Akker.

03:50-04:10 01.02.06  
Ligand-binding and Conformational Thermodynamics of Tryptophanyl-tRNA Synthetase (TrpRS). Maryna Kapustina, Charlie Carter.

04:10-04:30 01.02.07  
Structural Studies of *E. coli* Transhydrogenase A Multi-technique Approach for Membrane Proteins. Holly Heaslet, Mutso Yamaguchi, Vidyasankar Sundaresan, Mark Yeager, C. David Stout.

04:30-05:00 01.02.08  
Diversity of Conformational Epitopes on the Core Antigen of Hepatitis B Virus. David Belnap, Norman Watts, James Conway, Naiqian Cheng, Stephen Stahl, Paul Wingfield, Alasdair Steven.

### 03.01 Interface Between Powder and Single Crystal Diffraction

Columbus E-F Joe Reibenspies, Jim Britten, Presiding

*Acknowledgment is made to ICDD for partial support of this session.*

08:30-09:00 03.01.01  
Single Crystal Insights into Powders and Fibers - A Role for Electron Crystallography? Douglas L. Dorset.

09:00-09:30 03.01.02  
Crystal Structure of Guaiifenesin, 3-(2-methoxyphenoxy)-1,2-propanediol. James Kaduk.

09:30-10:00 03.01.03  
Structural Analysis of Chlorpropamide Polymorphs: A Potential Shear-based Phase Transformation. Peter Wildfong, Stephan Boerrigter, Simon Bates, Kenneth Morris.

10:00-10:30 Coffee Break.

10:30-11:00 03.01.04  
Structural Chemistry of Novel Bis(Oxalato)Borate Salts and their Solvates. Peter Y. Zavalij, M. Stanley Whittingham.

11:00-11:30 03.01.05  
Crystal Structures of Titanosilicates: Complimenting X-ray Powder Diffraction Techniques by Single Crystal Diffraction Methods. Akhilesh Tripathi, Dmitri G. Medvedev, Jose Delgado, Abraham Clearfield.

11:30-12:00 03.01.06  
Heeding Anisotropic "Powder" Patterns. Rob Grothe.

12:00-01:30 Lunch Break.

01:30-02:00 03.01.07  
Micro X-ray Powder Diffraction Using Loops. Nattamai Bhuvanesh, Joseph Reibenspies.

02:00-02:30 03.01.08  
Micro-diffraction: Versatility in X-ray Analysis. Ralph Tissot, Mark Rodriguez.

02:30-03:00 03.01.09  
Recent Work in OSU's Crystallographic Laboratories. Alex Yokochi.

03:00-03:30 Coffee Break.

03:30-04:00 03.01.10  
Simulations of Debye-Scherrer and Gandolfi Patterns Using a Bruker SMART/APEX Diffractometer System. Stephen Gugenheim.

04:00-04:30 03.01.11  
Powder Diffraction at the Advanced Photon Source: Now and Future. Peter Lee, Yuegang Zhang, Robert VonDreele.

04:30-05:00 03.01.12  
Microcrystal Diffraction with Synchrotron Radiation: When is a Powder not a Powder? William Clegg.

**Powder Diffraction SIG Meeting at 05:15pm**

**04.01 Frontiers in Single-Crystal Neutron Diffraction**

**Columbus C-D Art Schultz, Tom Koetzle, Presiding**

08:45-08:50 Opening Remarks.

08:50-09:25 04.01.01  
An Overview of the Spallation Neutron Source. Ian S. Anderson.

09:25-10:00 04.01.02  
Neutron Diffraction Studies on Metal Cluster Hydride Complexes. Robert Bau.

10:00-10:30 Coffee Break.

10:30-11:05 04.01.03  
Structure and Dynamics of Transition Metal Hydrides. Michael Heinekey, Tom Koetzle.

11:05-11:40 04.01.04  
Linear M-H-M Bonding in a Simple Dinuclear Metal Complex. David Vicic, Thomas Anderson, Curtis Berlinguette, Kim Dunbar, John Cowan, Arthur Schultz, Olav Schiemann, George Stanley.

11:40-01:30 Lunch Break.

01:30-02:05 04.01.05  
Skutterudites: Their Structural Response to Filling. Bryan Chakoumakos.

02:05-02:40 04.01.06  
Single-crystal Neutron Diffraction Studies of Hydrogen-bonded Proton Conductors. Calum Chisholm, Sossina Haile, Wim Klooster.

02:40-03:00 04.01.07  
The New Quasi-Laue Diffractometer at the Replacement Research Reactor. Wim Klooster.

03:00-03:30 Coffee Break.

03:30-03:50 04.01.08  
Progress Toward Thermal Neutron Laue Diffraction at the NCNR. Brian H. Toby, C.Y. Jones, A. Santoro, P.C. Brand, E. Prince, T.D. Pike, D.L. Jacobson.

03:50-04:10 04.01.09  
Neutron Diffraction Structure of Fully Deuterated Aldose Reductase: A Necessary Complement to X-ray Ultra-high Resolution Structures. Alberto Podjarny, Andre Mitschler, Isabelle Hazemann, Mathew Blakeley, Marie Therese Dauvergne, Flora Meilleur, Michael Van Zandt, Steve Ginell, Andrzej Joachimiak, Dean Myles.

04:10-04:30 04.01.10  
Preliminary Neutron Studies of Protocatechuate 3,4-Dioxygenase. Douglas H. Ohlendorf, C. Kent Brown, Paul Langan, Benno P. Schoenborn.

04:30-04:50 04.01.11  
Direct Methods and Macromolecular Neutron Diffraction. Herbert A. Hauptman, David A. Langs.

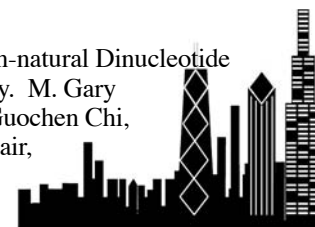
04:50-05:00 Closing Remarks.

**05.01 Important Bioorganic Science from Small Molecules**

**Columbus A-B John Desper, Presiding**

08:30-09:15 05.01.01  
Binding and Membrane Transport of Anions and Salts Using Synthetic Receptors. Bradley Smith.

09:15-09:30 05.01.02  
Structural Investigation of a Non-natural Dinucleotide with Anti-HIV Integrase Activity. M. Gary Newton, Charles F. Campana, Guochen Chi, Doowon Lee, Z. -J. Liu, Vasu Nair, James Phillips, John P. Rose, B.C. Wang.



09:30-09:45 05.01.03

Importance of Glu28 in the Protection of Thiamine Diphosphate in Benzoylformate Decarboxylase. Asim Kumar Bera, Natalie Anderson, Miriam S. Hasson.

09:45-10:00 05.01.04

A New Biological Insight for the Organic Compounds  $C_{16}H_{11}O_2N$ ,  $C_{17}H_{13}O_3N$  and  $C_{17}H_{13}O_4N$ . Helena Napolitano, R.H.A. Santos, A.B.F. Silva, L. Silva, R. Borges, C.N. Alves.

10:00-10:30 Coffee Break.

10:30-11:15 05.01.05

Interplay of Crystal Structures and Computational Methods in the Design of Bioactive Molecules. Olaf Wiest, DiFei Wang, Patrick Laine, Marco Jonas, Mickael Pauvert.

11:15-11:30 05.01.06

A New Structural Insight from Inhibition against *Leishmania major promastigotes*. Hamilton Napolitano, M. Silva, J. Elena, W.C. Rocha, P.C. Vieira, B.D.G. Rodrigues, A.L.C. Almeida, G. Oliva, O.H. Thiemann.

11:30-11:45 05.01.07

Crystal Structures of Two Anti-Cancer Quinolins and Models of their Thio redoxin Binding. Carl Schwalbe, Ruobo Ren, Dan Rathbone, Andrew Westwell, Malcolm Stevens.

11:45-12:00 05.01.08

Structural Preferences of N-substituted Monosaccharide Derivatives. William H. Ojala, S.E. Hanson, T.M. Skrypek, J.M. Smieja, R.J. Sabo, J.M. Ostman, C.R. Ojala.

## Small Molecule SIG Meeting at 05:15pm Columbus I-L

## X-Rays, Crystals, Molecules, and You

Grand Ballroom F Judy Flippen-Anderson, Presiding

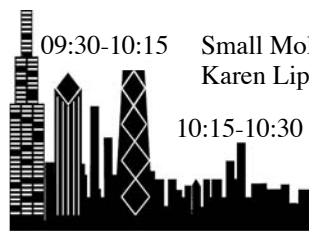
This workshop, designed for high school teachers and students, will include presentations on the general basics of crystallography, the wealth of information derived from crystallography contained in the databases that store 3-dimensional structural results and examples of how this data can be used in the classroom. Presentations will also include a description of existing programs involving high school teachers and students for the rapid prototyping of molecular models. There will be mini-workshops on growing protein crystals and building molecular models, as well as hands-on interaction with the databases. Several of the high school students have contributed posters that will be on display as part of the Sunday evening poster session.

08:30-08:45 Welcome. Judy Flippen-Anderson

08:45-09:30 Crystallography: The Nuts and Bolts. Katherine Kantardjieff.

09:30-10:15 Small Molecule Building Blocks. Karen Lipscomb.

10:15-10:30 Coffee Break.



10:30-11:15 The PDB and You. David Goodsell.

11:15 – 12:00 SMART Teams: Students Modeling a Research Topic. Tim Herman, Tommie Hata.

12:00 – 01:30 Lunch break.

01:30 – 04:30 *Teachers:* Lysozyme Crystal Growing Workshop. Alex McPherson. *Students:* Hands-on Model Building and Database Interaction. Tim Herman, David Goodsell, Karen Lipscomb

04:30 – 07:30 Commercial exhibits and Poster Session.

## AW.01 Margaret C. Etter Early Career Award Session

Columbus A-B

Bill Ojala, Mark Whitener, Presiding

01:30 Presentation of Award to Leonard Macgillivray. Fran Jurnak, ACA President.

01:30-02:30 AW.01.01  
Linear Templates: Tools for Constructing Molecules in the Solid State. Leonard MacGillivray.

02:30-02:50 AW.01.02  
Halogen Bonding: A Useful Tool for Crystal Design. William T. Pennington, Jeffrey L. Harris, Brian T. Holmes, Clifford W. Padgett, Timothy W. Hanks.

02:50-03:10 AW.01.03  
Supramolecular Structures of Triangles, Squares, Loops and Carceplexes Based on Metal-metal Bonded Units. Xiaoping Wang, F. Albert Cotton.

03:10-03:35 Coffee Break.

03:35-03:55 AW.01.04  
Use of Fluorinated Tetrphenylporphyrins for the Cocrystallization of Fullerenes. Marilyn Olmstead, Daniel Nurco.

03:55-04:15 AW.01.05  
Routine and Unusual Structures of Copper-Imidazole Complexes with Carboxylate Counter Ions. Mark Whitener, Mousumi Roy, Sandra Victorin, Jessica Kasner.

04:15-04:35 AW.01.06  
Understanding Coordination, Packing, and Hydrogen Bond Patterns of Metal Carboxylates. Graciela Diaz de Delgado.

04:35-04:55 AW.01.07  
Selenium Derivatization of Nucleic Acids and MAD Phasing for Structure Determination. Zhen Huang, Jiansheng Jiang, Nicolas Carrasco.

04:55-05:15 AW.01.08  
Chirality Comes Naturally: A Chiral 3D Nickel Aspartate Framework with Large One-dimensional Channels. Ekaterina Anokhina, Yongjae Lee, Thomas Vogt, Allan J. Jacobson.

# Monday, July 19

Council Meeting Room	07:30am	Grand Suite 5	Service Cr SIG Meeting	05:25pm	Columbus A-B
Speaker Ready Room	07:30am	Columbus H	Poster Session II	05:30pm	Riverside Center East
Interview Room	07:30	Columbus G	Rigaku/MSC Dinner	07:30pm	House of Blues (by invitation only)
Exhibit Show	10:00am	Riverside Center East	Young Scientist Mixer	07:30pm	Crystal Ballroom (pre-purchased ticket required)
Macromolecules SIG Meeting	05:15pm	Columbus I-L	<i>Thanks to Hampton Research, Nextal and Fluidigm for partial support of the Mixer</i>		
Neutron Scattering SIG Meeting	05:15pm	Columbus E-F			
General Interest SIG Meeting	05:15pm	Columbus C-D			

## TRANSACTIONS SYMPOSIUM

### TR.01 Crystals in Supramolecular Chemistry

Columbus E-F

Alicia Beatty, Presiding

#### Morning Session: Crystal Structure Prediction and Polymorphism

08:30-08:35 Opening Remarks, Alicia Beatty.

08:35-09:30 TR.01.01

Crystal Structure Prediction and Polymorphism - Some Mutual Insights. Sarah (Sally) L. Price, Binal Patel, Pinky Pridhanani Jethani, Antonio Torrisi.

09:30-10:00 TR.01.02

Polymorph "Prediction": Where Have We Been? Where Are We Now? Where Are We Going? Joel Bernstein.

10:00-10:30 Coffee Break.

10:30-11:00 TR.01.03

A New, Simple Description of Crystal Packing. Elna Pidcock, Sam Motherwell.

11:00-11:30 TR.01.04

A Journey Towards the Final Form of a 2nd Generation Drug Candidate of MaxiPost. Q. Gao, S.-M. Kuang, D. Wu, D. Provencal, J. Bien, C.-P. Chen, Y. Pendri, Y. Chen, S.-Y. Sit, K. Xie, K. Gillman, D. Bocchino, J.E. Starrett, Jr.

11:30-12:00 TR.01.05

Studies of Phase Relationships in Cocrystal Systems. Raymond E. Davis, Keith A. Lorimer, Matthew A. Wilkowsky, Jr., Joseph H. Rivers, Kraig A. Wheeler, Jeffrey Bowers.

12:00-01:45 Lunch Break.

#### Afternoon Session: Crystal Growth Mechanisms

01:45-02:45 TR.01.06

Test of Cairns-Smith's Crystals-as-genes Hypothesis. Bart Kahr, T. Bullard, S. Avagyan, M. Kurimoto.

02:45-03:15 TR.01.07

Uric Acid Crystal Growth. Jennifer A. Swift, Ryan E. Sours, Dorothy A. Fink, Kristin A. Cox, Catherine E. Ford.

03:15-03:45 Coffee Break.

03:45-04:15 TR.01.08

Patterned Crystals *via* Solvent-mediated Self-assembly. G. Tayhas Palmore, Tzy-Jiun Luo, John MacDonald.

04:15-04:45 TR.01.09

Designing Molecular Interfaces. Colin Seaton, Nick Blagden.

04:45-05:00 TR.01.10

Kinetic Resolution of Amino Acids in Natural and Modified Gels. Rositza Petrova, Rakesh Patel, Andrew Pogozelski, Jennifer Swift.

05:00-05:15 TR.01.11

Optical Probes of Growing Crystals: Elucidating Surface Chemistry and "Sensing" Polar Axes. Jason B. Benedict, A. Barbon, M. Bellinazzi, M. Brustolon, S.D. Fleming, S.-H. Jang, S. Lovell, B. Khar, A.L. Rohl.

*Session Continues on Tuesday, July 20, at 08:30am*

### 01.03 Computational Methods

Columbus I-L

Wayne Anderson, Paul Adams, Presiding

08:30-08:55 01.03.01

LABELIT: Robust Indexing for Automatic Data Collection. Nicholas Sauter, Ralf Grosse-Kunstleve, Paul Adams.

08:55-09:20 01.03.02

Structure Determination from Weak Anomalous Signals. George M. Sheldrick.

09:20-09:45 01.03.03

Automated Applications of BnPI. Methodology. William Furey, L. Pasupulati, S.A. Potter, H. Xu, R. Miller, C.M. Weeks.

09:45-10:05 01.03.04

MAIN in 2004: Model Building at 100 Residues per Minute. Dusan Turk.

10:05-10:35 Coffee Break.

10:35-11:00 01.03.05

Real Space Protein Model Completion: An Inverse Kinematics Approach. Henry van den Bedem, Itay Lotan, Jean-Claude Latombe, Ashley Deacon.

11:00-11:25 01.03.06

Beyond Engh and Huber: Towards Development of More Accurate Methodology in Macromolecular Crystal Structure Refinement. Thomas R. Transue, Joseph M. Krahn, Thomas A. Darden.

11:25-11:50 01.03.07

High Throughput Structure Determination: Exploring Different Software Paths. Joseph S. Brunzelle, Wayne F. Anderson.



## 01.04 Difficult Structures

**Columbus I-L**      **Todd Yeates, Dauter Zbigniew, Presiding**

01:45-02:15      01.04.01  
Crystal Structure of the Human  $\beta$ 2-Chimaerin Using SAD and Molecular Replacement. Bertram Canagarajah, Jonathan Ho, Layla Saidi, Marcelo Kazanietz, James Hurley.

02:15-02:45      01.04.02  
Yeast Copper Thionein: Solving a Small but Long-standing Puzzle. Vito Calderone, Benedikt Dolderer, Hans-Juergen Hartmann, Hartmut Echner, Claudio Luchinat, Cristina Del Bianco, Stefano Mangani, Ulrich Weser.

02:45-03:15      01.04.03  
A Problematic Case: Crystal Structure of Disintegrin Using Data from a Crystal with Pseudosymmetry. Sameeta Bilgrami, P. Kaur, S. Yadav, A.S. Ethayathulla, R. Prem Kumar, T. Ja-been, S. Sharma, M. Perbandt, Ch. Betzel, T.P. Singh.

03:15-03:45      Coffee Break.

03:45-04:15      01.04.04  
Crystal Structure of Streptococcus Pyogenes Mac-1 Exhibiting Twinning Problem. Agniswamy Johnson, Sergei Radaev, James Musser, Peter Sun.

04:15-04:45      01.04.05  
Structural Determination of a Partial Hemihedral Twinned Actin Crystal. Robbie Reutzler, Lakshmanan Govindasamy, Mavis Agbandje-McKenna, Robert McKenna.

04:45-05:15      01.04.06  
Crystallization and Preliminary Phasing of Recombinant Vaults. Daniel Anderson, Valerie Kickhoefer, Sujna Raval-Fernandes, Leonard Rome, David Eisenberg.

**Biological Macromolecules SIG Meeting 05:15pm**

## 02.03 Teaching Advanced Crystallography

**Columbus A-B**      **Peter Müller, Presiding**

01:45-01:55      Opening Remarks.

01:55-02:20      02.03.01  
Teaching Crystallography to Biologists. Jenny Glusker.

02:20-02:45      02.03.02  
When Less is More: Teaching Crystallography to Bioscientists. Bernhard Rupp.

02:45-03:10      02.03.03  
Making a MAD Experiment Seem Rational. Michael Sawaya.

03:10-03:45      Coffee Break.

03:45-04:10      02.03.04  
The BCA/CCG Intensive Teaching School in X-ray Structure Analysis. Robert Gould.

04:10-04:35      02.03.05  
Teaching about Problems of Disorder, Twinning and Pseudo-Symmetry. William Clegg.

04:35-05:00      02.03.06  
Crystallography after the Refinement. Larry R. Falvello.

05:00-05:25      02.03.07  
Some Useful Concepts in Teaching Structure Determination and Structural Chemistry. George M. Sheldrick.

**Service Cr SIG Meeting 05:25pm**

## 07.02 Macromolecular Crystal Quality and X-ray Diffraction

**Columbus C-D**      **Edward Snell, Presiding**

08:30-09:00      07.02.01  
Diffraction and Imaging Study of Imperfections of Protein Crystals with Coherent X-rays. Z.W. Hu, B.R. Thomas, A.A. Chernov, Y.S. Chu, B. Lai.

09:00-09:30      07.02.02  
Defects in Bio-Molecular Crystals as Seen by High-resolution X-ray Imaging. Vivian Stojanoff, B. Capelle, Y. Epelboin, J. Haertwig, A. Moraleda, F. Otalora.

09:30-10:00      07.02.03  
Effective Quality Improvement of  $\alpha$ -Amylase Crystals under Microgravity. Hiroaki Tanaka, Koji Inaka, Shigeru Sugiyama, Masaru Sato, Sachiko Takahashi, Satoshi Sano, Susumu Yoshitomi, Hiroshi Komatsu.

10:00-10:30      Coffee Break.

10:30-11:00      07.02.04  
Crystal Salvaging Efforts at SECSG. Jeff Habel, Ashit Shah, Zhi-Jie Liu, Jessie Chang, Sue Chang, Peter Horanyi, Angela Yang, Lisa Huang, John Rose, Bi-Cheng Wang.

11:00-11:30      07.02.05  
Winners and Losers - Ranking Crystals from Diffraction Images. Angela Criswell, Robert Bolotovskiy, Thaddeus Niemeyer, Russ Athay, James Pflugrath.

11:30-12:00      07.02.06  
High-pressure X-ray Crystallographic Studies of Viral Assemblies. Keith Brister, Roger Fourm, Mao Ho-kwang, John E. Johnson, Lin Tianwei.



## 08.03 Complementary Methods Using Synchrotron Radiation

Columbus A-B

Wayne Anderson, Presiding

*Acknowledgment is made to Structural GenomiX, Inc., for partial support of this symposium.*

08:30-09:00 08.03.01

Structure of Core-shell and Alloyed Binary Nanoparticles Studied with X-ray Absorption Fine Structure. Bruce Bunker, Debudutta Lahiri, Tomohiro Shibata, Zhenyuan Zhang, Soma Chattopadhyay, Jeff Terry, Dan Meisel.

09:00-09:30 08.03.02

Study of Magnetic Structures with Circularly Polarized Synchrotron Radiation. George Srajer, Daniel Haskel, Jonathan C. Lang, D.R. Lee, Y. Choi, D. Keavney, J.S. Jiang, J. Meerschaert, S.D. Bader, W.C. Uhlig.

09:30-10:00 08.03.03

Small and Wide-angle Scattering at ChemMatCARS: Bridging the Gap between 'Ideal' and 'Real' Materials. David Cookson, Myungae Lee, David Schultz.

10:00-10:30 Coffee Break.

10:30-11:00 08.03.04

Ultra-small-angle X-ray Scattering (USAXS) Imaging to Complement USAXS Analysis. Gabrielle Long, Lyle Levine.

11:00-11:30 08.03.05

Assigning Protein Fold on the Basis of Wide-angle Solution Scattering Data. Lee Makowski, Diane Rodi, Robert Fischetti.

11:30-12:00 08.03.06

Direct Measurements of Structure Factor Phases on Several Protein Structures. Andrew Stewart, Qun Shen.

## AW.02 Supper Symposium in Honor of Nguyen-Huu Xuong

Columbus C-D

K.I. Varughese, Andy Howard, Presiding

01:00 Presentation of Award to Nguyen-Huu Xuong. Frances Jurnak, ACA President.

01:00-01:45 AW.02.01

Advanced Area Detectors for Protein Crystallography and Electron Microscopy. Nguyen-Huu Xuong.

01:45-02:05 AW.02.02

The Evolution of Detectors Used for Protein Crystallography - A Personal Overview. Ronald Hamlin.

02:05-02:30 AW.02.03

The Evolution of Protein Crystallographic Detectors: Past, Present and Future. Edwin M. Westbrook.

02:30-02:50 AW.02.04

PILATUS 1M: A Single Photon Counting Pixel Detector for Protein Crystallography. Christian Broennimann, Eric Eikenberry, Gregor Huelsen.

02:50-03:15 AW.02.05

Photon Counting Detectors for Time-resolved X-ray Diffraction in Structural Biology. Gerd Rosenbaum.

03:15-03:45 Coffee Break.

03:45-04:15 AW.02.06

Detector Characteristics and Data Processing. J.W. Pflugrath.

04:15-04:45 AW.02.07

Detectors and Storage Rings. Andrew J. Howard.

04:45-05:15 AW.02.08

The Role of Detectors in Time-resolved Crystallography. Vukica Srajer.



## Tuesday, July 20

Council Meeting Room	07:30am	Grand Suite 5	Materials Science SIG Meeting	05:30pm	Columbus A-B
Speaker Ready Room	07:30am	Columbus H	Small Angle Scattering SIG Meeting	05:30pm	Columbus E-F
Interview Room	07:30am	Columbus G	Synchrotron Radiation SIG Meeting	05:15pm	Columbus I-L
Exhibit Show	10:00am	Riverside Center East	Young Scientist SIG Meeting	05:15pm	Columbus C-D
Lunch & Learn High-Throughput Crystallography - Accerlys/IBM	12:00pm	Gr Ballroom CD	Poster Session III	05:30pm	Riverside Center East
			Rigaku/MSC Fun	07:30pm	Hyatt Front Entrance

### TRANSACTIONS SYMPOSIUM

#### TR.01 Crystals in Supramolecular Chemistry Columbus E-F Alicia Beatty, Presiding

*Acknowledgment is made to the Donors of The American Chemical Society Petroleum Research Fund for partial support of this symposium.*

#### Morning Session: Crystal Structure Design

08:30-09:30 TR.01.12  
Molecular Tectonics: From Simple Tectons to Complex Molecular Networks. Mir Wais Hosseini.

09:30-10:00 TR.01.13  
From Molecular Function to Supramolecular Assembly. Christer Aakeröy, John Desper, Brock Levin, Janie Salmon, Nathan Schultheiss, Ben Scott, Michelle Smith, Joaquin Urbina.

10:00-10:30 Coffee Break.

10:30-11:00 TR.01.14  
Complementary Features of Inorganic and Organic Halogens - Application to Crystal Engineering. Lee Brammer, Fiorenzo Zordan, Guillermo Mínguez Espallargas, Stephen Purver, Luis Arroyo Marin, Harry Adams.

11:00-11:30 TR.01.15  
Can We use  $\pi$ - $\pi$  Interactions in the Designed Synthesis of Inorganic-organic Hybrid Materials? Jesus Valdes-Martinez, Ruben A. Toscano, Domingo Salazar-Mendoza, John Desper.

11:30-12:00 TR.01.16  
Engineering Molecular Crystals. James D. Wuest.

12:00-01:45 Lunch Break.

#### Afternoon Session: Applications of Crystal Design

01:45-02:45 TR.01.17  
Engineering Crystal Architecture Through Molecular Design: Applications of Supramolecular Assembly. Michael Ward.

02:45-03:15 TR.01.18  
Supramolecular Chemistry in Alternative Solvents: Are Non-volatile Ionic Liquids Effective Crystallization Solvents or Fodder for Co-crystals? Robin D. Rogers, Scott T. Griffin, Grant A. Broker, W. Matthew Reichert, Jane H. Poplin, Richard P. Swatloski, John D. Holbrey.

03:15-03:45 Coffee Break.



03:45-04:15 TR.01.19  
Making, Using, Transforming Crystals: An Hydrogen Bonded Material that Reacts with Vapours and Crystals. Dario Braga, Fabrizia Grepioni, Lucia Maini, Marco Polito, Stefano Giaffreda, Katia Rubini.

04:15-04:45 TR.01.20  
Symmetry and Crystal Design. Joseph Lauher, Frank Fowler.

04:45-05:15 TR.01.21  
Metal-organic Polygons, Polyhedra, and Extended Frameworks Derived from Molecules Constructed in the Solid State. Leonard MacGillivray, Giannis Papaefstathiou, Tamara D. Hamilton, Qianli Chu, Tomislaav Friscic

#### 01.05 New Structures Columbus I-L Todd Yeates, Zbigniew Dauter, Presiding

08:30-08:55 01.05.01  
Structural Basis for the Inhibition of the Carboxyltransferase Domain of Acetyl-coenzyme A Carboxylase. Hailong Zhang, Zhiru Yang, Yang Shen, Tweel Benjamin, Liang Tong.

08:55-09:20 01.05.02  
The Structure of the N-terminal Domain of Lis1 Reveals a Novel and Ubiquitous Dimerization Motif. David Cooper, Myung Hee Kim, Arkadiusz Oleksy, Yancho Devedjiev, Urszula Derewenda, Orly Reiner, Jacek Otlewski, Zygmunt Derewenda.

09:20-09:45 01.05.03  
Structure of the C-terminal Domain of Prokaryotic Topoisomerase II: A Novel  $\beta$ -Propeller Implies How Gyrase Wraps DNA. Nei-Li Chan, Tung-Ju Hsieh.

09:45-10:05 01.05.04  
Crystal Structure of a Self-splicing Group I Intron from Phage Twort. Barbara Golden, Elaine Chase.

10:05-10:35 Coffee Break.

10:35-10:55 01.05.05  
First Structure of a Bi-functional Proline Catabolic Enzyme. John Tanner, Jonathan Schuermann, Dale Karr, John Larson.

10:55-11:20 01.05.06  
Crystal Structure of the Human Cytosolic Sialidase Neu2: Evidence for the Dynamic Nature of Ganglioside Recognition. Leonard Chavas, Paolo Fusi, Cristina Tringali, Bruno Venerando, Guido Tettamanti, Ryuichi Kato, Eugenio Monti, Soichi Wakatsuki.

11:20-11:45 01.05.07  
The Structure of the APPBP1-UBA3-NEDD8-ATP Complex Reveals the Basis for Selective Ubiquitin-like Protein Activation by an E1. Helen Walden, Michael Podgorski, Brenda Schulman.

## 06.01 General Interest I

Columbus C-D

Alex Yokochi, Presiding

01:45-02:15 06.01.01

If Physics Doesn't Work, Try Math: Understanding Chemistry Using Graph Theory. David Brown.

02:15-02:45 06.01.02

Electron Density Distribution in Crystals: New Results in Understanding the Nature of Chemical Bonding. Mikhail Yu. Antipin, Konstantin A. Lyssenko.

02:45-03:15 06.01.03

Fabrication of Complex Crystals Using Kinetic Control, Chemical Additives and Epitaxial Growth. John MacDonold, G. Tayhas R. Palmore, Tzy-Jiun Mark Luo.

3:15-03:45 Coffee Break.

03:45-04:05 06.01.04

Advances in X-ray Optics: Improving the Performance of Sealed Tube Based Diffraction Systems. Anita Coetzee, Bram Schierbeek, Arjen Storm.

04:05-04:25 06.01.05

New Developments in Chromium Phasing. Cheng Yang, J.W. Pflugrath, A. Yamano, H. Kawasaki, H. Yamazaki, C.N. Stence, A.D. Courville, J.D. Ferrara.

04:25-04:55 06.01.06

Combinatorial Optimization Algorithms for the Phase Problem in Single-crystal X-ray Diffraction. Anastasia Vaia, Nikolaos Sahinidis.

04:55-05:15 06.01.07

Moonlighting Proteins. Constance Jeffery.

## 09.01 Topics for Young Scientists

Columbus C-D

Chad Haynes, Matthew Clifton, Presiding

08:30-08:40 Opening Remarks. Arwen Pearson, SIG Chair.

08:40-09:20 Interviewing Skills. J. Ferrara, RigakuMSC.

09:20-10:00 The National Postdoctoral Association: A New Resource for Young Scientists. Alyson Reed, Executive Director, National Postdoctoral Association.

10:00-10:30 Coffee Break.

10:30-10:50 Career Choice: Academia. Frances Jurnak, Univ. of California, Irvine.

10:50-11:30 Intellectual Property and Patents. Nabeela McMillian, Marshall, Gerstein and Borun LLP.

11:30-11:50 Careers in Industrial Crystallography? Jim Kaduk, BP Chemicals.

11:50-12:00 Closing Remarks. Chad Haynes, SIG Chair Elect

**Young Scientists SIG Meeting 05:15pm**

## 10.01 Materials for the 21st Century

Columbus A-B

Brent Heuser, Jason Hodges, Presiding

**Morning Session Chair: Brent Heuser**

08:30-09:00 10.01.01

Supramolecular Self Assemblies of Variants of Amyloid Peptides. P. Thiyagarajan, Kun Lu, Jijun Dong, Jaby Jacob, Vincent Conticello, David Lynn.

09:00-09:30 10.01.02

Dynamical Responses in Polymer-Clay Solutions. Paul Butler, Matthew Malwitz, Lionel Porcar, Sheng Lin-Gibson, Gudrun Schmidt.

09:30-10:00 10.01.03

Damage Accumulation in Si During He and Self-ion Implantation. Y. Zhong, P. Partyka, R.S. Averback, S.K. Ghose, I.K. Robinson.

10:00-10:30 Coffee Break.

10:30-11:10 10.01.04

A Chemist's Perspective to Heavy Fermion Intermetallics. Robert T. Macaluso, Robin Macaluso, Willa Williams, Julia Chan.

11:10-11:35 10.01.05

Structural and Magnetic Characterization of the Perovskite Type 112 Compounds, REBaCuCoO<sub>5+δ</sub> (RE = rare earths and Y). Leopoldo Suescun, Alvaro Mombrú, Camille Jones, Brian Toby, Claudio Cardoso, Fernando Araújo-Moreira.

11:35-12:00 10.01.06

Large Force Ceramic Actuators for Smart Systems. Waltraud M. Kriven.

12:00-01:45 Lunch Break.

**Afternoon Chair: Jason Hodges**

01:45-02:30 10.01.07

Noncentrosymmetric Inorganic-organic Materials. Kenneth Poepelmeier.

02:30-03:15 10.01.08

Superstructures in Polytelluride Compounds with Square Nets: Are They "Everywhere"? Mercuri Kanatzidis.

03:15-03:45 Coffee Break.

03:45-04:25 10.01.09

Reticular Synthesis and the Design of New Materials. Omar Yaghi.

04:25-04:50 10.01.10

A Series of Novel Materials: Gallium and Aluminium Propylene-diphosphonate. Zhanhui Yuan, Martin Attfield, William Clegg.

04:50-05:05 10.01.11

Total Scattering: The Structural Technique for the 21st Century. Thomas Proffen.

05:05-05:30 10.01.12

The Upgraded General Purpose Powder Diffractometer at IPNS-ANL. J.W. Richardson, Jr. E. Maxey, Y. Li, A. Huq.

**Materials Science SIG Meeting 05:30pm**



**AW.03 Fankuchen Award Symposium in Honor of Alexander McPherson**

**Columbus I-L Bob Cudney, George DeTitta, Presiding**

01:00 Presentation of Award to Alexander McPherson. Frances Jurnak, ACA President.

01:00-01:45 AW.03.01  
Where Are We Going, Where Have We Been? Alexander McPherson.

01:45-02:15 AW.03.02  
Protein Crystallization in the Year Twenty-two AM: What Have We Learned From High Throughput Crystallization and Structural Genomics We Did Not Know Before? Bernard Rupp.

02:15-02:45 AW.03.03  
Ions from the Hofmeister Series: Effects on Proteins in Solution and in the Crystallization Process. Kim Collins.

02:45-03:15 AW.03.04  
Crystallization Strategy in the Midwest Center for Structural Genomics. Youngchang Kim, Irina Dementieva, Ruiying Wu, Min Zhou, Grazyna Joachimiak, Lour Lezondra, Pearl Quartey, Hui Li, Andrzej Joachimiak.

03:15-03:45 Coffee Break.

03:45-04:15 AW.03.05  
The Design of Self-Assembled 3D DNA Crystals. Nadrian Seeman, Pamela Constantinou, Baoquan Ding, Tong Wang, Jens Kopatsch, Ruojie Sha, Jens Birktoft, Furong Liu, Robert Sweet, Chengde Mao.

04:15-04:45 AW.03.06  
A Pragmatic Approach to Automation and High Throughput Crystallography in a Pharmaceutical Setting. William Somers, Joel Bard, Kristine Svenson, Ercolani Kimberly.

04:45-05:15 AW.03.07  
Integrated Fluidic Circuits: The New Paradigm for Protein Crystallization. Kyle Self, Andrew May, Susanna Ng.

**Small Angle Scattering SIG Meeting 05:30pm Columbus E-F**

**Synchrotron Radiation SIG Meeting 05:15pm Columbus I-L**

**EVENING SESSIONS**

**Plans for the NIH Protein Structure Initiative**

**Columbus A-B Judy Flippen Anderson, Presiding**  
08:00pm - 09:30pm

The NIH recently announced its plans for the next phase of the Protein Structure Initiative (PSI). Beginning in 2005, this production phase will comprise an interacting network with three components: large-scale research centers, specialized research centers focused on methods development and challenging proteins, and disease-targeted research centers (pending). At the ACA workshop, John Norvell, director of the PSI, will describe the project and will summarize the two recent Requests for Applications (RFAs) that will support the first two components of the PSI.

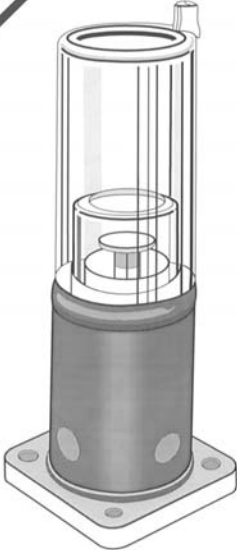
**02.02 Crystallographic Laboratory Practices**

**Columbus C-D Alicia Beatty, Presiding**  
08:00pm - 09:30pm

This session aims to be an informal, hopefully informative and enjoyable, panel discussion concerning issues that come up in the service laboratory. It will cover such subjects as publishing, authorship, charges for services, general laboratory practices. Refreshments will be served.

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
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# Wednesday, July 21

Council Meeting Room	07:30am	Grand Suite 5	Poster removal completed by	03:30pm	Riverside Center East
Speaker Ready Room	07:30am	Columbus H	ACA All Member Business Meeting	05:00pm	Columbus E-F
Interview Room	07:30am	Columbus G	<b>Annual Awards Banquet</b>		<b>Crystal Ballroom</b>
Exhibit Show	10:00am	Riverside Center East	Cash Bar	06:30pm	(pre-purchased ticket only)
ACA Canadian Div. Meeting	12:00pm	Columbus I-L	Dinner	07:30pm	

## 01.06 Membrane Structures

**Columbus I-L Michael Wiener, Declan Doyle, Presiding**

08:30-09:00 01.06.01

Structure of the Translocation Unit of a Bacterial Autotransporter. Piet Gros, Clasiën Oomen, Peter van Ulsen, Patrick van Gelder, Maya Feijen, Jan Tommassen.

09:00-09:15 01.06.02

Purification and Crystallization of Membrane Proteins Involved in Type IV Pilus Biogenesis. Liliana M. Sampaleanu, Patrick Yip, Lori L. Borrows, P. Lynne Howell.

09:15-09:30 01.06.03

Investigating the Role of Protein and Surfactant Interactions in Membrane Protein Crystallization. Bryan Berger, Colleen Gendron, Gabriella Santonicola, Clifford Robinson, Eric Kaler, Abraham Lenhoff.

09:30-10:00 01.06.04

X-ray Structure of a Protein-conducting Channel. William M. Clemons, Bert Van Den Berg Jr., Ian Collinson, Yorgo Modis, Enno Hartmann, Stephen C. Harrison, Tom A. Rapoport.

10:00-10:30 Coffee Break.

10:30-11:00 01.06.05

Crystal Structure of Cyanobacterial Photosystem II. Tina M. Iverson, Kristina N. Ferreira, Farim Maghlaoui, Jim Barber, So Iwata.

11:00-11:15 01.06.06

Structures of Photosynthetic Reaction Center Mutants that Influence Proton Transfer. Marianne Schiffer, Deborah Hanson, Phil Laible, S. Ginell, Raj Pokkuluri.

11:15-11:30 01.06.07

Time-resolved Crystallographic Studies of Light-induced Structural Changes in the Photosynthetic Reaction Center. Richard Baxter, Nina Ponomarenko, Vukica Srajer, Reinhard Pahl, Keith Moffat, James Norris.

11:30-12:00 01.06.08

Selectivity of Organic Transmembrane Channel Families. Robert Stroud.

## 01.07 Macromolecular Assemblies

**Columbus I-L Wei Yang, Stephen Sprang, Presiding**

01:30-02:00 01.07.01

SNARE Selectivity of the COPII Coat. Lincoln Bickford, Elena Mossessova, Jonathan Goldberg.

02:00-02:30 01.07.02

Structural and Functional Implications of the Heterodimeric GTPase Latch that Docks SRP to its Receptor. Douglas Freymann, Irina Shepotinovskaya, Pamela Focia.

02:30-02:55 01.07.03

Inhibitor Binding Induced Conformational Changes in the Cytochrome bc<sub>1</sub> Complex Suggest a Mechanism for the Capture-and-release of the Iron-sulfur Protein Subunit. Di Xia, Lothar Esser, Chang-An Yu.

02:55-03:25 Coffee Break.

03:25-03:55 01.07.04

Helical Bundle Conversion: Structural Alterations as Relays in Integrin Signaling. Tina Izard, Gwyndaf Evans, Robert A. Bor-gon, Christina L. Rush, Clemens Vornrhein, Gerard Bricogne, Philippe RJ Bois.

03:55-04:25 01.07.05

Cryo-EM and X-ray Crystallographic Studies on the Mono-meric Kinesin Motor KIF1A. Masahide Kikkawa.

04:25-04:50 01.07.06

Crystal Structure of the SeqA-N Fiber: Implications for DNA Replication and oriC Sequestration. Alba Guarne, Therese Brendler, Qinghai Zhao, Rodolfo Ghirlando, Stuart Austin, Wei Yang.

## 05.02 Combining Spectroscopy, Calculations, and Crystallography for Solving Chemical Problems

**Columbus E-F Alberto Albinati, Larry Falvello, Presiding**

08:30-09:00 05.02.01

The Use of Neutron Elastic Scattering for the Investigation of Dynamic Processes in Disordered Systems and Biological Materials. Antonio Deriu.

09:00-09:30 05.02.02

X-ray Crystallography and NMR Spectroscopy: Two Partners Separated by a Solvent. Paul Pregosin, Silvia Rizzato.

09:30-10:00 05.02.03

Study of High-Spin Hindered Imidazole Iron(II) Porphyrinate Complexes. W. Robert Scheidt, Chuanjiang Hu, Arne Roth, Mary Ellison, Jin An, Charles Schulz.

10:00-10:20 Coffee Break.

10:20-10:50 05.02.04

Synergy between Neutron Scattering Experiments and Computational Studies on Sorbates in Porous Materials. Juergen Eckert.

10:50-11:20 05.02.05

Separating Electronic, Steric, and Packing Interactions in Crystallographic Structures by Density Functional Theory. Michael B. Hall, Charles Edwin Webster.



11:20-11:50 05.02.06

Crystallization-Induced Asymmetric Transformations and Chiral Organometallics. Jack Faller, Nikos Sarantopoulos.

11:50-12:10 05.02.07

Computer Program for Ligand Solid Angle Calculations. Iliia Guzei.

## 05.03 Non-routine Refinement of Small Molecules

Columbus C-D

Vic Young, Presiding

08:30-09:00 05.03.01

The Absolute Structure of 2,2''-Dimethoxy-[1,2';4',1'';3'',1''']quarter-naphthalene-3',2''-diol, C<sub>42</sub>H<sub>30</sub>O<sub>4</sub>(EtOAc): A Merohedrally Twinned and Disordered Structure. Michal Sabat, Marilise A. Hyacinth, Charles F. Campana, George M. Sheldrick.

09:00-09:30 05.03.02

(CH<sub>3</sub>)<sub>3</sub>N-CB<sub>10</sub>H<sub>12</sub> - A Commensurately Modulated Carbaborane Compound. Charles Campana, Ludger Häming, John Huffman.

09:30-10:00 05.03.03

Molecule Symmetry and Crystallographic Disorder. Jeffrey Deschamps, Damon Parrish, Nurulain Zaveri.

10:00-10:30 Coffee Break.

10:30-11:00 05.03.04

Translational Disorder and Crystal Growth Mechanisms in Channel Inclusion Compounds. Mark Hollingsworth, John Bacsá, Charles Campana, Matthew Peterson.

11:00-11:30 05.03.05

Looking for Hydrogen Atoms in X-ray Data. Bruce Noll, Thomas Fehlner, Sundargopal Ghosh, Hong Yan.

11:30-12:00 05.03.06

Multipole Refinement of High-resolution X-ray Diffraction Data: Characterizing a Weak Through-space Interaction in a Peri-substituted Naphthalene. Christopher S. Frampton, Leo Straver, John Wallis.

## 06.02 General Interest II: Cool Structures

Columbus A-B

Allen Oliver, Presiding

01:30-01:55 06.02.01

Intercalation Compounds of the  $\gamma$ -zirconium Phosphate: X-ray Characterization. Carla Ferragina, Romolo Di Rocco, Lucantonio Petrilli.

01:55-02:20 06.02.02

Local and Long Range Symmetry in Ferroelastic Lead Phosphate at High Pressure. Ross Angel, Ulrich Bismayer, William Marshall.

02:20-02:45 06.02.03

Crystal Structure of Potato Tuber ADP-glucose Pyrophosphorylase. James Geiger, Xiangshu Jin, Jack Preiss.

02:45-03:10 06.02.04

An Example of High Order Oligomeric Protein Assembly. Mirosław Gilski, Dominika Borek, Zbyszek Otwinowski.

03:10-03:30 Coffee Break.

03:30-03:55 06.02.05

Crystal Engineering of Thermostable Acentric Crystals. Tatiana Timofeeva, Vladimir Nesterov, Volodymyr Nesterov, Mikhail Antipin.

03:55-04:20 06.02.06

Theoretical Modeling of Crystal Structures of Three Polymorphs of N, N-dimethyl-4-nitroaniline. Tiffany Kinnibrugh, Tatiana Timofeeva.

04:20-04:45 06.02.07

X-ray Diffraction Analysis of "Ionic Liquids": What Can We Learn More about Ionic Liquid Solution? Konstantin Lysenko, Denis Golovanov, Mikhail Antipin, Alexander Shaplov, Yakov Vygodskii.

04:45-05:10 06.02.08

The Unusual Phases of Anhydrous and Hydrated Pinacol. Carolyn P. Brock, Xiang Hao, Sean Parkin.



## 07.01 Biological Macromolecules: Solution Behavior and its Relation to Crystallization Columbus C-D Patrick Loll, Presiding

01:30-02:00 07.01.01  
Does the Anisotropy of Intermolecular Interactions Determine the Protein Crystal Symmetry? Peter Vekilov.

02:00-02:30 07.01.02  
Protein/polyethylene Glycol Phase Behavior: Implications for Protein Crystallization. Denis Vivares, Eric Kaler, Abraham Lenhoff.

02:30-03:00 07.01.03  
Aggregated Pre-crystallization State of Ferritin Seen by Solution Scattering at Low Temperature. Sebastien Boutet, Ian Robinson.

03:00-03:30 Coffee Break.

03:30-04:00 07.01.04  
Small-Angle Neutron Scattering Studies of PEG/Protein Solutions under Crystallization Conditions. Susan Krueger, Ken Rubinson, Dobrin Bossev, Gary Gilliland.

04:00-04:30 07.01.05  
Platform for Protein Crystallization Studies: Screening and Optimization *via* Control of the Supersaturation Rate. Paul Kenis, David Kim, Sameer Talreja, Charles Zukoski.

04:30-05:00 07.01.06  
Extrapolating Crystallization Conditions and Improving Reproducibility in Protein Crystal Growth: Theory, Experiment and Technology. Viatcheslav Berejnov, Robert Thorne.

## 11.01 Ultra Small-angle Scattering Science Columbus A-B Peter J. Jemian, Presiding

08:30-09:00 11.01.01  
Pore Morphology of Membrane Filters. Dale Schaefer, A'reum Kim, Kumar Chokalingam, Ryan Justice, Max Belfor.

09:00-09:20 11.01.02  
Microstructure of Dense Colloidal Suspensions and Gels. Subramanian Ramakrishnan, Yeng Long Chen, Syed Ali Shah, Kenneth Schwiezer, Charles Zukoski.

09:20-09:40 11.01.03  
Structure of Polymer-nanocomposites - A USAXS Study. R. A. Narayanan, P. Thiyagarajan, B.J. Ash, S.S. Sternstein, A.J. Zhu, L. Schadler.

09:40-10:00 11.01.04  
Micron Pores in Vycor Porous Glass: Evidences from USANS. Yuri Melnichenko, G.D. Wignall, D.R. Cole, M. Agamalian, I. Pozdnyakova, D. Schwahn, H. Frielinghaus, A. Radulescu, E. Kentzinger.

10:00-10:30 Coffee Break.

10:30-10:50 11.01.05  
Combined USANS/SANS Measurements in Archaeometry. Roberto Triolo, Fabrizio Lo Celso, Irene Ruffo, Valerio Benfante, Carlo Gorgoni, Paolo Pallante.

10:50-11:10 11.01.06  
*In situ* USAXS Studies of Nucleation and Particle Growth in the Flame Aerosol Process. Nikhil Agashe, Greg Beaucage, Hendrik Kammler, Rainer Jossen, Pete Jemian, Sotiris Pratsinis.

11:10-11:30 11.01.07  
Morphology of Polymer/LC Composites. Ryan Justice, Tim Bunning, Rich Vaia, Dale Schaefer.

11:30-12:00 11.01.08  
Characterization of Poly (N-isopropylacrylamide) Gels by Ultra-small Angle Scattering. Vijay R. Tirumala, L. Guo, P. Thiyagarajan, J.G. Barker, G.T. Caneba, D.C. Mancini.

*Session Continues on Thursday, July 22, at 08:30am*

## AW.04 Trueblood Award Symposium in Honor of Richard E. Marsh Columbus E-F Jenny Glusker, Presiding

*Acknowledgment is made to the Donors of The American Chemical Society Petroleum Research Fund for partial support of this symposium.*

01:30 Presentation of Award to Richard Marsh. Frances Jurinak, ACA President.

01:30-02:30 AW.04.01  
X-ray Diffraction Through the Years: From One Structure per Year to One Structure per Hour. Richard E. Marsh.

02:30-03:00 AW.04.02  
First Order Enantiotropic Solid State Phase Transitions - From Simon through Ubbelohde to Mnyukh`. Frank H. Herbststein.

03:00-03:30 Coffee Break.

03:30-04:00 AW.04.03  
Molecular Motion in Crystals. Hans-Beat Bürgi.

04:00-04:30 AW.04.04  
Hydrogen Bonding, Graph Sets, Co-crystals and Crystal Design. Joel Bernstein.

04:30-05:00 AW.04.05  
Problems/Solutions Encountered in Crystallographic Analyses of Nanosized Metal Carbonyl Clusters. Lawrence Dahl, Guy-ét Tran, Evgueni Mednikov, Namal de Silva, Sergei Ivanov, Rita Nichiporuk, Michael Kozee.

*Session Continues on Thursday, July 22, at 08:30am*



Council Meeting Room	07:30	Grand Suite 5	Interview Room	07:30	Columbus G
Speaker Ready Room	07:30	Columbus H			

## 01.08 Structural Bioinformatics

**Columbus I-L Ram Samudrala, Daniel Fischer, Presiding**

08:30-09:05 01.08.01  
Quality Assurance in Structural Bioinformatics. Philip Bourne.

09:05-09:40 01.08.02  
Rational Genomics: Sense/Antisense Open Reading Frames and the Amino Acid Composition of Ribosomal Proteins. W. L. Duax, J. Schaber, L. Habegger, R. Huether, V. Pletnev, S. Connare.

09:40-10:15 01.08.03  
Automatic Protein Structure Prediction for Structural Genomics: ORFans, the 3D-SHOTGUN Meta-predictor Approach and CAFASP. Daniel Fischer.

10:15-10:45 Coffee Break.

10:45-11:20 01.08.04  
Automated Interpretation of NMR Data Using Structures Derived from X-ray Crystallography. Ling-Hong Hung, Ram Samudrala.

11:20-11:55 01.08.05  
Delaunay Tetrahedral Decomposition Structural Alignment. Jeffrey Roach, Shantanu Sharma, Charles W. Carter, Jr.

## 01.09 Fresh Approaches to Express and Purify Biomolecules

**Columbus I-L Song Tan, Alex Edwards, Presiding**

01:30-02:00 01.09.01  
Total Chemical Synthesis of Proteins for Crystallographic Structure Determination: Current Status, Future Promise. Stephen Kent.

02:00-02:30 01.09.02  
Auto-induction for Protein Production in Inducible T7 Expression Systems. F. William Studier.

02:30-03:00 01.09.03  
Evaluation of High Throughput Methods for Cloning and Expression of Soluble Domains. Frank Collart, Shiu Moy, Lynda Dieckman, Elizabeth Landorf, Terese Pepler, Natalia Maltsev, Fred Stevens, Marianne Schiffer.

03:00-03:30 Coffee Break.

03:30-04:00 01.09.04  
Strategies to Improve Protein Expression and Solubility: Lessons from the Structural Genomics of Plasmodium. Sujata Sharma, Jocelyne Lew, Peter Loppnau, Farrell Mackenzie, Anthony Semesi, Adelinda Yee.

04:00-04:30 01.09.05  
Production of Eukaryotic Proteins for High-throughput Structure Determination. George Phillips.

04:30-05:00 01.09.06  
Purification of the Holo-TFIID Complex from *Saccharomyces cerevisiae* for Structural Studies. Raymond Jacobson.

## 06.03 General Interest III: Advances in Computing Environment for Crystallography

**Columbus A-B Lachlin Cranswick, Presiding**

01:30-02:00 06.03.01  
BnP on the Grid. Russ Miller, M.L. Green, C.M. Weeks.

02:00-02:30 06.03.02  
GRID-enabled Structure Determination from Powder Diffraction Data. Anders Markvardsen, Kenneth Shankland, Bill David.

02:30-03:00 06.03.03  
Coot: Model Building Tools for Protein Crystallography. Paul Emsley.

03:00-03:30 Coffee Break.

03:30-04:00 06.03.04  
User Friendly Software for Single Crystal, TOF Neutron Scattering Data Visualization and Reduction. Dennis Mikkelsen, A. Schultz, R. Mikkelsen, P. Peterson, T. Worlton, J. Hammonds, J. Cowan, M. Miller, C. Bouzek, M. Miller.

04:00-04:30 06.03.05  
CrystMol 2.1 - New Tools for Analysis of Multiple Determinations of the Same or Similar Structures. David Duchamp.

## 08.01 Radiation Damage I: Site & Wavelength Specificity; Limits to Dose and Sample Size

**Columbus C-D Gerd Rosenbaum, Presiding**

*Acknowledgment is made to Structural GenomiX, Inc., for partial support of this symposium.*

08:30-08:40 Introduction. Gerd Rosenbaum.

08:40-09:10 Report from 3rd International Workshop on X-ray Damage to Biological Crystalline Samples: Summary of Papers Relevant to Session 08.01. Elspeth Garman.

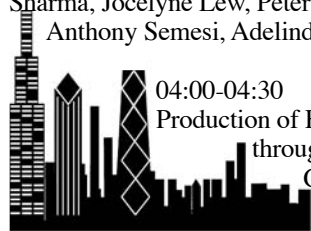
09:10-09:40 08.01.01  
Can We Beat Radiation Damage? Mehmet Aslantas, J. Jakoncic, M. DiMichiel, V. Honkimaki, Z. Zhong, V. Stojanoff.

09:40-10:00 08.01.02  
Dehydration and Collapse of Protein Crystals. Ian Robinson, Sebastien Boutet.

10:00-10:30 Coffee Break.

10:30-11:00 08.01.03  
What Time-resolved ESR Tells us About the Radiolytic Oxidation of Amino Acids in Solution. Gordon L. Hug, Pawel Wisniewski, Ian Carmichael, Richard W. Fessenden.

11:00-11:30 08.01.04  
At Which Level of Flux Density Can One Expect Dose Rate to Matter. Gerd Rosenbaum.



**08.02 Radiation Damage II: Extracting Maximum Information from Limited Sample Life**  
**Columbus C-D**                      **Gerd Rosenbaum, Presiding**

*Acknowledgment is made to Structural GenomiX, Inc. for partial support of this symposium.*

01:30-02:00      Introduction to Session 08.02 and Report from 3rd International Workshop on X-ray Damage to Biological Crystalline Samples: Summary of Papers Relevant to Session 08.02. Gerd Rosenbaum.

02:00-02:30      08.02.01  
 The Effects of Energy and Crystal Composition on the Radiation Dose Absorbed by Macromolecular Crystals. Elspeth Garman, James Murray, Raimond Ravelli.

02:30-03:00      08.02.02  
 A Multi-Data-Set Data Collection Strategy Using Dose Derived Exposures for Optimum Data Acquisition. Z.J. (James) Liu, L.R. Chen, G. Rosenbaum, J. Chrzas, Z.-Q Fu, J. Rose, B.C. Wang.

03:00-03:30      Coffee Break.

03:30-04:00      08.02.03  
 Correcting Radiation Damage in Macromolecular Diffraction Data by Statistical Methods. Zbyszek Otwinowski, Dominika Borek, Wladek Minor.

04:00-04:30      08.02.04  
 Phasing in the Presence of Severe Site-Specific Radiation Damage Through Dose-Dependent Modeling of Heavy Atoms. Marc Schiltz, P. Dumas, G. Bricogne.

04:30-05:00      08.02.05  
 Single Crystal SIR/SIRAS: Exploitation of Radiation Damage for Macromolecular Phasing. Udipi Ramagopal, Thirumuran Radhakannan, Steven Almo.

**11.02 Ultra Small-angle Scattering Techniques**  
**Columbus E-F**                      **Peter J. Jemian, Presiding**

08:30-09:00      11.02.01  
 Versatile USAXS (BONSE-HART) Facility for Advanced Materials Research. Jan Ilavsky, Pete R. Jemian, Andrew J. Allen, Gabrielle G. Long.

09:00-09:30      11.02.02  
 Performance of a Thermal-Neutron Double-crystal Diffractometer for USANS at NIST. Paul Butler, John Barker, James Moyer, Man-Ho Kim, Andrew Drews, Michael Agamalian, Charles Glinka

09:30-10:00      11.02.03  
 Application of Spin-echo Small-angle Neutron Scattering in Colloidal Systems. Wim G. Bouwman, Timofei V. Krouglov, Jeroen Plomp, Serguei V. Grigoriev, Wicher H. Kraan, M. Theo Rekveldt.

10:00-10:30      Coffee Break.

10:30-10:45      11.02.04  
 A Method for Polarization Control and Analysis on BONSE-HART Double-crystal USANS Instruments. Kenneth Littrell, Wai Tung Lee.

10:45-11:05      11.02.05  
 A Method for Analysing Multiple Scattering in SANS and USANS Data Using Matching Fourier Transforms. Willem Bertram.

11:05-11:25      11.02.06  
 Satoshi Koizumi.

11:25-11:45      11.02.07  
 A Time-of-Flight Ultra-Small-Angle Neutron Scattering Instrument Performance Gain Over its Reactor-Based Analog. Michael Agamalian, John M. Carpenter, Kenneth C. Littrell, Alexandry Stoica, Christine Rehm, Pappannan Thiagarajan.

11:45-12:05      11.02.08  
 Test Experiments of TOF-USANS for the JSNS. Kazuya Aizawa, Tetsuya Yokoo, Masatoshi Arai.

**AW.04 Trueblood Award Symposium in Honor of Richard E. Marsh**  
**Columbus A-B**                      **Emily Maverick, Presiding**

*Acknowledgment is made to the Donors of The American Chemical Society Petroleum Research Fund for partial support of this symposium.*

08:30-09:00      AW.04.06  
 Structures of New Au-N Compounds. The Shortest Au-Au bond and Characteristic Au-Au Interactions in Dinuclear and Tetranuclear Complexes. John P. Fackler Jr., Hanan Abdou, Ahmed A. Mohamed.

09:00-09:30      AW.04.07  
 Lattice-dynamical Modelization of Physical Properties of Crystals. Carlo Maria Gramaccioli.

09:30-10:10      AW.04.08  
 Analysis and Illustration of Thermal Motion Covariance. Carroll K. Johnson, Michael N. Burnett.

10:10-10:30      Coffee Break.

10:30-10:50      AW.04.09  
 The Hazards of Using Space Groups of Too High Symmetry. Frank Fronczek.

10:50-11:15      AW.04.10  
 Marshing: Past, Present and Future. Anthony Spek.

11:15-11:40      AW.04.11  
 Metal Ions in Biological Systems: Information from Crystallographic and Theoretical Studies. Jenny Glusker, Amy Katz, Charles Bock.

11:40-12:00      AW.04.12  
 Mogul - Rapid Retrieval of Molecular Geometry from the Cambridge Structural Database. G.M. Battle.



# POSTERS

## Manned Poster Sessions

Riverside Center East

**Sunday, July 18 05:30pm - 07:30pm**

refreshments sponsored in part by Rigaku/MSU

**Monday, July 19 05:30pm - 07:30pm**

refreshments sponsored in part by 3-D Pharmaceuticals

**Tuesday, July 20 05:30pm - 07:30pm**

## Posters:

- Will be up Sunday - Wednesday on 4ft. x 4ft. boards
- Should be assembled between 10:00am-05:00pm on Sunday
- Should be removed between 12:00-03:30p.m. on Wednesday
- Numbers including PP, indicate candidates for the Pauling Prize
- Numbers including an X indicate candidates for the Oxford Prize

### P001 Poster Session III

Crystal Structure of the Broadly Cross-reactive HIV-1 Neutralizing Human Monoclonal Antibody Reveals Multiple Conformations of the CDR H3 Loop. Ramalakshmi Darbha, Yijun Gu, Michelle Andrykovitch, Meiyun Zhang, Dimiter S. Dimitrov, Xinhua Ji.

### P002 Poster Session I

Unusual Pseudo-nine-fold Rotational Symmetry in Crystals of the *Panulirus interruptus* Clottable Protein. Justin Kollman, Russell Doolittle.

### P003 Poster Session III

Algebraic Direct Methods for Very Low Resolution Protein Structure Determination. D.Y. Guo, Robert H. Blesing.

### PP004 Poster Session I

Comparison of Amyloid Fiber Diffraction Data with Structural Computational Models. Janel W. Laidman, Michael R. Sawaya, Todd O. Yeates.

### P005 Poster Session III

Investigation Aminosaccharides and their Derivative Properties by Molecular Modeling Method. A.M. Levkovich, S.S. Rashidova, N.L. Voropaeva, I.N. Ruban.

### P006 Poster Session II

Structure Solution for SF-1 by Combined SAD Phasing from the Sulfur Anomalous Signal with Molecular Replacement. Kevin P. Madauss, C. Yang, D. Juzumiene, S. Williams, J.D. Ferrara.

### PP007 Poster Session II

PyrR- Evolution of an RNA-binding Transcriptional Attenuation Protein. Preethi Chander, R.L. Switzer, J.L. Smith.

### P008 Poster Session III

A Structural Comparison of CBS Domains. Marianne Cuff, Rongguang Zhang, Tatiana Skarina, Alexei Savchenko, Aled Edwards, Andrzej Joachimiak.

### P009 Poster Session III

Repression of Human Nuclear Receptor LXR-1 Signaling by SHP. Eric Ortlund, Isaac Solomon, Matthew Redinbo.

### P010 Poster Session II

Automated Data Processing at SGX-CAT. John Badger, Jon Christopher, Thomas Peat, Wasserman Stephen.

### P011 Poster Session III

Rasy and Ras Indices for Evaluating the Anomalous Scattering Signal to Noise Level. Zheng-Qing Fu, John Rose, Bi-Cheng Wang.

### P012 Poster Session II

Application Programming with Crystallographic Concept/Protocol Libraries (CCL/CPL). Zhong Ren, Xiaojing Yang, Wayne Anderson.

### P013 Poster Session III

Stereochemical Rules for Connecting Disjoint Protein Fragments. Andrzej Kudlicki, Maga Rowicka, Zbyszek Otwinowski.

### P014 Poster Session II

Automation for Solving Protein Structures. Graeme Winter, C.C. Ballard, P.J. Briggs.

### P015 Poster Session III

Protein Model Validation in Structural Genomics - The SECSG Perspective. Wolfram Tempel, Z.J. Liu, W.B. Arendall, III, S.R. Wang, D.C. Richardson, J.S. Richardson, J. Rose, B.C. Wang.

### P016 Poster Session II

Phasing of Isomorphous Replacement Data Based on a Subset of Strongest Reflections. Yanina Vekhter.

### P017 Poster Session III

Novel Statistical Approach to the Phase Problem. Hongliang Xu, Herbert A. Hauptman.

### P018 Poster Session II

SGXPRO: A Versatile Structure Solving Engine for Structural Biology/Genomics. Bi-Cheng Wang, Fu Zheng-Qing, Wu Yunzhou, Che Dongsheng, Zhao Jizhen, Yan Haijin, Rose John.

### P019 Poster Session II

A High Throughput Pipeline for Protein-ligand Complex Crystal Structure Determination. Jian Xu, Zeljko Dzakula, Dan Berard.

### PP020 Poster Session II

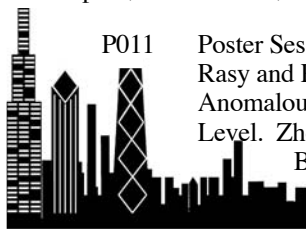
Understanding Color Vision in Mammals: X-ray Crystal Structures of Some Cellular Retinoic Acid Binding Protein II Mutants as a Mimic of Rhodopsin. Soheila Vaezeslami, Erika Mathes, Chrysoula Vasileiou, Rachael M. Crist, James H. Geiger, Babak Borhan.

### P021 Poster Session III

Crystal Structure of a Quinohemoprotein Alcohol Dehydrogenase ADH-IIG from *Pseudomonas putida* HK5. Zhi-wei Chen, F. Scott Mathews, Hirohide Toyama, Megumi Fukumoto, Megumi Yano, Osao Adachi, Kazunobu Matsushita.

### P022 Poster Session II

Preliminary Structural Studies of MauG, a Novel di-heme Protein Involved in Tryptophan Tryptophylquinone (TTQ) Biogenesis. A.R. Pearson, Y. Wang, M.E. Graichen, T. De La Mora-Rey, A. Liu, V.L. Davidson, C.M. Wilmot.



P023 Poster Session III

Difficult Structure for Interesting Reason - *E. coli* YfbU Gene Product. Dominika Borek, Yuanhong Chen, Mingzhu Zheng, Zbyszek Otwinowski.

PP024 Poster Session I

Analytical Ultracentrifugation as a Method to Analyze Membrane Protein Homogeneity. Matthew C. Clifton, Huide Zhang, John W. Burgner, II, Mark A. Hermodson, Cynthia V. Stauffacher.

P025 Poster Session II

The Challenging Structure Determination of Tomato Fruit Polygalacturonase: Space Group Ambiguity Arising from Pseudo-symmetry. Susan Heffron, Stephan Watkins, Rhonda Moeller, Aise Huma Taban, Rafal Butowt, Dean DellaPenna, Frances Jurnak.

P026 Poster Session III

Detection and Overcoming of Hemihedral Twinning During the MIRAS Structure Determination of rna1p. Roman C. Hillig, Louis Renault.

P027 Poster Session II

MCSG Case Study - A Difficult Structure Determination for yFCE, a Predicted Phosphoesterase from *E.coli*. Darcie Miller, Ludmilla Shuvalova, Elena Evdokimova, Alexei Savchenko, Alexander Yakunin, Wayne Anderson.

P028 Poster Session III

Intricate Crystal Structure of Dihydrolipoamide Dehydrogenase (E3) with its Binding Protein: Multiple Copies, Dynamic and Static Disorders. Anna Makal, Young Soo Hong, Rachel Potter, Amantha K. Vettaikorumakankauv, Lioubov G. Korotchkina, Mulchand S. Patel, Ewa Ciszak.

PP029 Poster Session I

The Structure of Phytanoyl-CoA Hydroxylase, an Fe(II), 2-oxoglutarate Dependent Dioxygenase Critical to Phytanic Acid Metabolism. Lindsay Odell, Jim C. Morrell, Stephen J. Gould, L. Mario Amzel.

P030 Poster Session II

Protein Crystallization by Surface Entropy Reduction: Novel Crystal Structures Showcase its Utility. Yogesh Surendranath, Izabela Janda, Yancho Devedjiev, Urszula Derewenda, Maksymilian Chruszcz, Wladek Minor, Andrzej Joachimiak, Zygmunt Derewenda.

PPX031 Poster Session I

Activation of *Cyanidium caldarium* RUBISCO. Michael Baranowski, Boguslaw Stec.

PPX032 Poster Session II

Comparison of Inhibitor Binding Modes to Aldose Reductase at Subatomic Resolution. Tatiana Petrova, Federico Ruiz, Andre Mitschler, Isabelle Hazemann, Alberto Podjarny, Michael Van Zandt, Steve Ginell, Andrzej Joachimiak.

P033 Poster Session II

Proton Transfer in Human Carbonic Anhydrase II: Effects of pH and Position of the Proton Shuttle Residue on the Transfer Rate. Suzanne Fisher, J. Hernandez, C.-K. Tu, D. Duda, C. Yoshioka, H. An, L. Govindasamy, D. Silverman, R. McKenna.

P034 Poster Session I

Crystallographic Studies of Phosphoenolpyruvate Carboxylase from *Anaerobiospirillum succiniciproducens*. Julien Coatesage, Louis Delbaere, Gregory Zeikus, Maris Laivenieks.

P035 Poster Session I

Structural Basis for Broad Neutralization by Anti-HIV-1 Antibody 447-52D. Robyn Stanfield, Mirosław Gorny, Constance Williams, Susan Zolla-Pazner, Ian Wilson.

P036 Poster Session III

Evolution of Function in the Family of Cyclitol Sugar Phosphatases. Boguslaw Stec, Kimberly Stieglitz, Mary Roberts.

P037 Poster Session III

Evolutionary Links in the Metabolic Synthesis/degradation of Nucleotides. Olga Mayans, Marco Marino, Miriam Deuss, Dmitri Svergun, Sterner Reinhard.

P038 Poster Session I

Structural Studies of Homologous Cytochromes c7 Involved in Fe(III) Reduction by *G. sulfurreducens*. Raj Pokkuluri, Yuri Londer, Xiaojing Yang, Norma Duke, George Johnson, Jill Erickson, Valerie Orshonsky, Marianne Schiffer.

P039 Poster Session II

The SECSG Protein-to-structure Pipeline: Potential and Limitations. John Rose, Zhi-Jie Liu, Dawei Lin, Wolfram Tempel, Lirong Chen, Gary Newton, Jane Richardson, Dave Richardson, Joseph Ng, Bi-Cheng Wang.

P040 Poster Session III

From Gene to Protein Automatically. A Platform Technology for Systematic, Automated and High Throughput Protein Expression and Purification. Grant Cameron, Robert Mount, Kevin Auton.

P041 Poster Session III

A Medium-throughput Approach to Optimal Protein Construct Generation with Difficult to Crystallize Proteins. Todd Geders, Larisa Avramova, Janet Smith.

PP042 Poster Session I

High-throughput Protein Production for Macromolecule Co-crystallization. Ashwini Nadkarni, Cory Momany, Laura-lee Clancy Kelley.

P043 Poster Session III

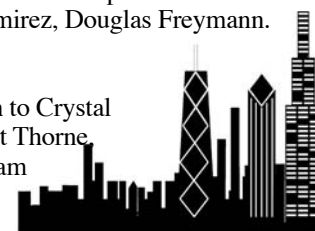
High Throughput Methods for Gene Expression and Purification of Hyperthermophilic *Pyrococcus furiosus* Proteins. Laura-Lee Kelley, Bret Dillard, Claudia Shah, Frank Sugar, Han-Seung Lee, Farris Poole, Francis Jenney, Jr., Michael Adams, Bi-Cheng Wang.

PPX044 Poster Session I

Water in the Structure-function Relationship of the SRPGTPase at 1.1 Å Resolution. Ursula Ramirez, Douglas Freymann.

P045 Poster Session II

MicroMounts: A New Approach to Crystal Handling and Mounting. Robert Thorne, Zachary Stum, Jan Kmetko, Adam Bartnik.



P046 Poster Session III

Structural Studies of Gas Binding in *Hansenula Polymorpha* Copper Amine Oxidase. B.J. Johnson, B.J. Brazeau, D.L. Wertz, J. Klinman, C.M. Wilmot.

P047 Poster Session II

Pico- and Femtomolar Transition State Inhibitor-complexes of MTA/AdoHcy Nucleosidase. J.E. Lee, V. Singh, V.L. Schramm, G.B. Evans, P.C. Tyler, R.H. Furneaux, P.L. Howell.

P048 Poster Session III

FiberNet: Developments in the Research Coordination Network for Biological Fiber Diffraction. Joseph Orgel, Rengaswami Chandrasekaran, Thomas Irving, Daniel Kirschner, Jianpeng Ma, Trevor Forsyth, John Squire, Gerald Stubbs.

P050 Poster Session III

Lipid Binding in Rice Nonspecific Lipid Transfer Protein-1 Complexes from *Oryza sativa*. Yuh-Ju Sun, Hui-Chun Cheng, Pei-Tsung Cheng, Peiyu Peng, Ping-Chiang Lyu.

P051 Poster Session II

Low Birefringence Plates for Crystal Scoring with Polarized Light. Ulrike Honisch, Guenther Knebel.

P052 Poster Session III

Anaerobic and Aerobic Structures of Ferredoxin II from *Desulfovibrio Gigas* Reveal Novel Electron Transfer Mechanism. Chun-Jung Chen, Yin-Cheng Hsieh, Ming-Yih Liu, Jean LeGall.

P053 Poster Session III

Studies of Tyrosyl-DNA Phosphodiesterase: Vanadate as a Tool for Exploring Mechanism, Macromolecular Assemblies and Inhibitor Design. Douglas Davies, Heidrun Interthal, James Champoux, Wim Hol.

P054 Poster Session I

Intermediate States Toward Two Functional Forms of Ribonuclease III in Complex with Double-stranded RNA. Jianhua Gan, Joe E. Tropea, Don Court, David S. Waugh, Xinhua Ji.

P055 Poster Session III

SANS Reveals that Protein Kinase A RI $\alpha$  Dimer Undergoes a Large Conformational Change upon Binding C Subunits. William Heller, Dominoco Vigil, Simon Brown, Donald Blumenthal, Susan Taylor, Jill Trehwella.

P056 Poster Session III

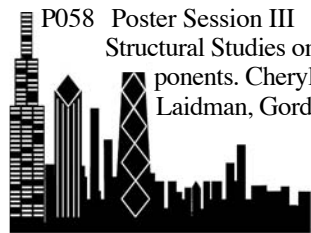
Structural Basis of Membrane-induced Cardiotoxin A3 Oligomerization. Chwan-Deng Hsiao, Farhad Forouhar, Wei-Ning Huang, Jyung-Hurng Liu, Kun-Yi Chien, Wen-guey Wu.

P057 Poster Session I

Crystal Structure of a Chimeric ATP Sulfurylase. Eric Lansdon, Irwin Segel, Andrew Fisher.

P058 Poster Session III

Structural Studies on Carboxysomes and their Components. Cheryl Kerfeld, Michael Sawaya, Janel Laidman, Gordon Cannon, Todd O. Yeates.



P059 Poster Session III

Crystal Structure of a Rad51 Filament. Phoebe Rice, Adam Conway, Thomas Lynch, Ying Zhang, Gary Fortin, Lorraine Symington.

P060 Poster Session III

Structures of the Human Topoisomerase I-DNA Covalent Complex Bound to Three Classes of Anticancer Agents. Bart Staker, Michael Feese, Mark Cushman, Yves Pommier, David Zembower, Lance Stewart, Alex Burgin.

P061 Poster Session III

The Interleukin-2 Receptor: Studies en Route to a Structure. D. J. Stauber, P.A. Horton, I.A. Wilson.

P062 Poster Session III

$\gamma$ 1-Adaptin Recognizes a [F/W]xx $\phi$  Motif of Accessory Proteins and the Hinge Region of GGA1. Yusuke Yamada, Masato Kawasaki, Ryuichi Kato, Kazuhisa Nakayama, Soichi Wakatsuki.

P063 Poster Session II

Cell Wall Biosynthesis, Folate Retention and Motility: Diverse Roles for a Common Enzyme Scaffold. Clyde Smith, Taru Deva, Edward Baker.

P064 Poster Session III

Inter-domain Signaling in Histidine Biosynthesis. Nagarajan Venugopalan, R.S. Meyers, V.J. Davisson, J.L. Smith.

P065 Poster Session III

Towards Structures of Membrane Proteins in 2D Crystals Using X-ray Free Electron Lasers. Michael Becker, Edgar Weckert.

PP066 Poster Session I

Preliminary X-ray Analysis of BphC1, an Extradiol Dioxygenase from *Sphingomonas* Strain BN6. Patrick Miller, Kiira Rattia, Andrew Mesecar.

P067 Poster Session III

Protein-Protein Interactions: Crystal Structures of Methotrexate-linked Dimers in Complex with *E. coli* Dihydrofolate Reductase. Vivian Cody, Kim Chisum, Jim Pace, C.R. Wagner, J.C.T. Carlson.

PP068 Poster Session I

The Crystal Structure of Factor Va: A New Mechanism for Membrane Binding and Function. Ty Adams, Matthew Hockin, Kenneth Mann, Stephen Everse.

PP069 Poster Session II

Decoding the Phenazine Biosynthesis Pathway: Structural Characterization of the Proteins PhzA & G from *Pseudomonas fluorescens* 2-79. Ekta Ahuja, Dimitri Mavrodi, Linda Thomashow, Wulf Blankenfeldt.

P070 Poster Session III

The Crystal Structure of Fms1 Reveals the Substrate Specificity of Polyamine Oxidase. Qingqui Huang, Qun Liu, Quan Hao.

P071 Poster Session I

A New Construct of Human Deoxycytidine Kinase Crystallizes in Multiple Complexes Allowing a More Complete View of Substrate Binding. Michael Godsey, Arnon Lavie.

P072 Poster Session II

A Thiamin-Bound, Pre-decarboxylation, Reaction Intermediate Analogue for Pyruvate in the Pyruvate Dehydrogenase Multi-enzyme Complex E1 Component. P. Arjunan, A. Brunskill, W. Furey, N. Nemeria, F. Jordan.

P073 Poster Session I

Structure Basis for Molecular Mechanism of MANT-GTP Inhibition of Mammalian Adenylyl Cyclase. Tung-Chung Mou, Andreas Gille, Roland Seifert, Stephen Sprang.

P074 Poster Session II

The Receptor Binding Site Architecture of Type IV Pilins Suggests a Mechanism for Conserved Receptor Specificity Despite High Sequence Diversity. Gerald Audette, Randy Irvin, Bart Hazes.

P075 Poster Session III

Crystal Structures of Familial ALS SOD1 Mutant G85R. Xiaohang Cao, Sai Seetharaman, Alexander B. Taylor, P. John Hart.

P077 Poster Session I

The Structure of NTBC Bound to 4-Hydroxyphenylpyruvate Dioxygenase. June Brownlee, Kayunta Johnson-Winters, David Harrison, Graham Moran.

PPX078 Poster Session II

Structure of the Group B *streptococcus* Surface Protein C5a Peptidase. C. Kent Brown, Zu-yi Gu, Yury Matsuka, P. Patrick Cleary, Stephen Olmstead, Douglas H. Ohlendorf, Cathleen A. Earhart.

P079 Poster Session III

Crystal Structures of Two 4-OT Homologues from *Helicobacter pylori* and *Archaeoglobus Fulgidus*. Rakhi Dasgupta, Jeffrey Almud, William Johnson, Chris Whitman, Marvin Hackert.

P080 Poster Session I

Crystal Structure of an Archaeal Peptidyl-tRNA Hydrolase from *Thermoplasma acidophilum*. Jerzy Osipiuk, Elena Evdokimova, Alexei Savchenko, Aled Edwards, Andrzej Joachimiak.

PPX081 Poster Session II

Purification and Crystallization of the Periplasmic Tripeptide Binding Protein MppA from *E. coli*. Forum Bhatt, Vishal Patel, Constance Jeffery.

P082 Poster Session I

Large-scale Motion of the Ligand Binding Domain of Nikkomycin Synthase. Chris Carrell, David Venci, Robert Bruckner, Marilyn Jorns, F. Scott Mathews.

P083 Poster Session III

Structures of Sortase B from *Staphylococcus aureus* and *Bacillus anthracis* Reveal Catalytic Amino Acid Triad in the Active Site. Andrzej Joachimiak, Rongguang Zhang, Ruiying Wu, Grazyna Joachimiak, Sarkis Mazmanian, Dominique Misiak, Piotr Gornicki, Olaf Schneewind.

PX084 Poster Session II

Crystal Structure of the p115RhoGEF rgRGS Domain in Complex with G $\alpha$ 13:G $\alpha$ i1 Chimera: A Novel G Protein GAP Mechanism. Zhe Chen, William D. Singer, Paul C. Sternweis, Stephen R. Sprang.

P085 Poster Session I

Crystal Structures of Conserved Hypothetical Protein YLBA from Three Different Bacteria. A.A. Fedorov, E.V. Fedorov, S.C. Almo.

PPX086 Poster Session II

Crystal Structure of a Biologically Active Peptide Complexed with G-Protein  $\beta$ : $\gamma$  Subunits. Tara Davis, Tabettha Bonacci, Alan Smrcka, Stephen Sprang.

P087 Poster Session I

Structure and Function of the GDNF Coreceptor  $\alpha$ 1. Adrian Goldman, Veli-Matti Leppänen, Maxim M. Bespalov, Pia Runeberg-Roos, Ülo Purand, Andres Merits, Mart Saarma.

PP088 Poster Session II

Unique Zinc Coordination by the C-terminal Domain of SecA. Brian Dempsey, Mark Wrona, Jana Moulin, Greg Gloor, Fari-dehj Jalilehvand, Gilles Lajoie, Gary Shaw, Brian Shilton.

P089 Poster Session III

The First High Resolution Crystal Structure of an Editosome Enzyme from *Trypanosoma brucei*: RNA Editing Ligase I. Junpeng Deng, Achim Schnauffer, Reza Salavati, Kenneth Stuart, Wim Hol.

P090 Poster Session I

Structure of Adeno-associated Virus Serotype 4. Lakshmanan Govindasamy, Eric Padron, Robert Mckenna, Nikola Kaludov, John.A Chiorini, Mavis-Agbandje Mckenna.

P091 Poster Session III

Structural Basis for Allosteric Regulation of the Monomeric Allosteric Enzyme Human Glucokinase. Kenji Kamata, Morihiro Mitsuya, Teruyuki Nishimura, Jun-ichi Eiki, Yasufumi Nagata.

PX092 Poster Session II

Crystal Structure of the Toll/interleukin-1 Receptor (TIR) Domain of Human IL-1RAPL. Javed Khan, Elizabeth Brint, Luke O'Neill, Liang Tong.

PX093 Poster Session I

Structure of Human dCK Suggests Strategies to Improve Anticancer and Antiviral Therapy. Elisabetta Sabini, Stephan Ort, Christian Monnerjahn, Manfred Konrad, Arnon Lavie.

PPX094 Poster Session II

Crystal Structure of 2,3-Dihydroxybiphenyl 1,2-Dioxygenase from *Rhodococcus globerulus* P6 and its Implications. Mustafa Koksal, Amparo Haro, Lindsay D. Eltis, Jeffrey T. Bolin.

P095 Poster Session III

Structural Analysis Reveals Determinants of Substrate Specificity of Biphenyl Dioxygenases. Pravindra Kumar, Christopher L. Colbert, Nathalie Agar, Cheryl Whiting, Emma Master, Lindsay Eltis, Justin Powloski, Jeffrey T. Bolin.

P096 Poster Session II

The Structure of a CH2-Deleted Humanized Antibody. Steven Larson, John Day, Alexander McPherson, Scott Glaser, Gary Braslawsky.



PX097 Poster Session I

YbdK is a Carboxylate-amine Ligase with  $\gamma$ -glutamyl: Cysteine Ligase Activity. Christopher Lehmann, Victoria Doseeva, Sadhana Pullalarevu, Wojciech Krajewski, Andrew Howard, Osnat Herzberg.

P098 Poster Session II

Crystal Structure of the Heterodimerization Complex Between Pals1-L27n Domain and Patj L27 Domain. Yuanhe Li, David Karnak, Ben Margolis, Arnon Lavie.

P099 Poster Session I

High Resolution Crystal Structure of a Putative Bacterial Lysozyme from *Bacillus stearothermophilus*. G. Minasov, J.S. Brunzelle, L. Shuvalova, S.F. Moy, F.R. Collart, W.F. Anderson.

P100 Poster Session II

Structure of Phosphoglycerate Mutase from *M. Tuberculosis* New Features. Peter Müller, Mike Sawaya, Sum Chan, Yim Wu, Inna Pashkova, Jeanne Perry, David Eisenberg.

P101 Poster Session I

Structural Study of Tomato Chloroplastic Cu,Zn Superoxide Dismutase. Susan T. Thomas, Amir Liba, Alexander B. Taylor, Aram M. Nersissian, Joan S. Valentine, P. John Hart.

PPX102 Poster Session II

Regulation of Nitrogen Metabolism in *Bacillus subtilis*: X-ray Crystal Structure of Glutamine Synthetase. David Murray, Lewis Wray, Jr., Susan Fisher, Richard Brennan.

P103 Poster Session I

Crystal Structures of Wild-type and Mutant (E261Q) of Long-chain Acyl-CoA Dehydrogenase With and Without Substrate Respectively. Beena Narayanan, H.K. Lee, A.W. Strauss, R. Paschke, J.-J.P. Kim.

PPX104 Poster Session II

Activation Mechanism and NAD-Binding Mode of Cholera Toxin are Revealed by Structural Studies of a Y30S Variant. Claire O'Neal, Edward Amaya, Michael Jobling, Randall Holmes, Wim Hol.

PP105 Poster Session I

The Structure of Allene Oxide Synthase from *Plexaura homomalla*, a Catalase-like Fold. Michael Oldham, Alan Brash, Marcia Newcomer.

P106 Poster Session II

The First Reported Crystal Structure of a Plant 5-enolpyruvylshikimate 3-phosphate Synthase (EPSPS)-Petunia EPSPS. T.J. Rydel, N. Leimgruber, H.S. Shieh, R.A. Stegeman, W.C. Stallings. G.S. Bild J.R. Borgmeyer Q.K. Huynh.

PX107 Poster Session I

Crystal Structure of Penicillin-binding Protein (PBP) Related Factor A from *Bacillus subtilis*. Thirumuruhan Radhakanann, Udipi Ramagopal, Steven Almo.

P108 Poster Session I

Crystal Structure of *T. fusca* Xyloglucanase (Glycosyl Hydrolyase Family 74). Joshua Sakon, David Wilson, Daniel Lincoln.

PP109 Poster Session II

Structure of PITP $\beta$  in Complex with Phosphatidylcholine: Comparison to Other PITP Isoforms. Paul B. Vordtriede, Chuong Doan, Jacque Tremblay, Lynwood R. Yarbrough, Marilyn D. Yoder.

PP110 Poster Session I

Understanding the Structural Basis for Amyloid Fiber Formation of Ribonuclease A. Shilpa Sambashivan, Yanshun Liu, David Eisenberg.

P111 Poster Session III

High Resolution Crystal Structures of the C-Fragment of Tetanus Toxin Heavy Chain. Macy Shen, K.A. Kantardjieff, B. Segelke, M. Knapp, B. Rupp, Sean Parkin.

P112 Poster Session I

Structural Studies of Human Mitochondrial Tryptophanyl tRNA Synthetase. Christopher J. Siemer, Charles W. Carter, Jr., Laurie S. Kaguni, Carol L. Farr.

P113 Poster Session II

The Structure of the Angiogenesis Inhibitor Angiostatin Bound to a Peptide from the Group A Streptococcal Surface Protein PAM. Sara Weaver, James Geiger.

PX114 Poster Session I

Structure of the Topoisomerase Domain of a Novel Archaeal Type IB Topoisomerase at 2.25 Å Resolution. Bhupesh Taneja, Aelxei Slesarev, Alfonso Mondragon.

PPX115 Poster Session II

Crystal Structure of Human DJ-1, a Protein Associated with Early-onset Parkinson's Disease. Xiao Tao, Liang Tong.

PX116 Poster Session I

Structures of HMG-CoA Synthase Complexes Reveal Mechanistic Details. Michael J. Theisen, Ila Misra, Dana Saadat, Henry M. Mizioro, David H. T. Harrison.

P117 Poster Session III

Structure of Yellow Fever Virus Helicase. Jinhua Wu, Richard Kuhn, Janet Smith.

P118 Poster Session I

The Structure of *Thermatoga maritima* S-adenosylmethionine Decarboxylase: Evidence for Gene Duplication and Fusion in the Evolution of AdoMetDCs. Angela Toms, Cynthia Kinsland, Anthony Pegg, Steven Ealick.

PX119 Poster Session II

RIa Subunit of PKA: A cAMP-free Structure Reveals a Hydrophobic Capping Mechanism for Docking cAMP into Site B. Jian Wu, Simon Brown, Nguyen-Huu Xuong, Susan Taylor.

P120 Poster Session III

The High Resolution Structure and Function of Cytochrome P450 (CYP158A2) from *S. coelicolor* A3(2). Bin Zhao, Michael Waterman.



P121 Poster Session I

Structure of *Mycobacterium tuberculosis* PyrR: A Persistence Gene and Drug Target. C. Vasquez, K. A. Kantardjieff, B-S. Rho, B. W. Segelke, T. Terwilliger, B. Rupp.

PP122 Poster Session II

Structure of *E. coli* AMP Nucleosidase Reveals Similarity to Nucleoside Phosphorylases. Yang Zhang, Sarah E. Cottet, Steven E. Ealick.

P123 Poster Session I

Crystal Structure of Filamentous Hemagglutinin Secretion Domain. Vincent Villeret, Bernard Clantin, H el ene Hodak, Eve Willery, Camille Loch, Fran oise Jacob-Dubuisson.

PPX124 Poster Session II

Crystal Structure of Aminoimidazole Riboside Kinase from *Salmonella enterica*. Yan Zhang, Diana Downs, Steve Ealick.

PP125 Poster Session I

Crystallization of Human Choline Acetyltransferase. Aeri Kim, R. J. Rylett, B. H. Shilton.

P126 Poster Session II

Crystallographic Screen for DNA Holliday Junctions. Franklin Hays, Amy Teegarden, Zebulon Jones, Dustin Raap, P. Shing Ho.

P127 Poster Session III

Comparison of Glycosyltransferases GtfA and GtfD for the Biosynthesis of Vancomycin Group Antibiotics: Ligand Binding and Regiospecificity. Anne Mulichak, Wei Lu, Heather Losey, Christopher Walsh, R. Michael Garavito.

PX128 Poster Session I

Crystal Structure of Putative Phosphomannomutase from *Thermus thermophilus* HB8. Shintaro Misaki, Kenji Suzuki, Naoki Kunishima, Mitsuaki Sugawara, Chizu Kuroishi, Masanori Kobayashi, Shoko Fujimoto, Masahiro Sakurai, Kazumi Nishijima.

PP129 Poster Session II

Structure Determination of the ATP Synthase Peripheral Stalk. Paul A. Del Rizzo, Brian H. Shilton, Stanley D. Dunn.

PPX131 Poster Session II

Conformational Flexibility of UDP-GlcNAc Pyrophosphorylase. Cynthia Sides, Jeffrey Wilson, Joshua Sakon.

PP132 Poster Session I

$\delta$ -Crystallin: A Model to Study the Enzymatic Mechanism of Argininosuccinate Lyase. May Tsai, Liliana Sampaleanu, Louise Creagh, Charles Haynes, P. Lynne Howell.

PP133 Poster Session II

Structural Studies of Pyruvoyl-Dependent Arginine Decarboxylase from *Methanococcus jannaschii*. Erika Soriano, Steve Ealick.

P134 Poster Session III

The Influencer of Second Component on the Structure and Crystallinity Degree of the Blends on the Base of Polysaccharide and Synthetic Polymer. Esma Ismailova, N.L. Voropaeva, N.D. Burkhanova, S.M. Yugay, G.V. Nikonovich, S.S. Rashidova.

PPX135 Poster Session II

Human Carboxylesterase 1: Structural Insights into a Multifunctional Bioscavenger. Christopher D. Fleming, S. Bencharit, Christopher L. Morton, Escher L. Howard-Williams, Phillip M. Potter, Matthew R. Redinbo.

PX136 Poster Session II

Human Carboxylesterase 1 in Cholesteryl Ester Hydrolysis and Atherosclerosis. Sompop Bencharit, Christopher L. Morton, Escher L. Howard-Williams, Peter Kuhn, Philip M. Potter, Matthew R. Redinbo.

PPX137 Poster Session I

Catching Catalysis in the Act: Using Single Crystal Kinetics to Trap Methylamine Dehydrogenase Reaction. Teresa De La Mora-Rey, Arwen R. Pearson, Kevin T. Watts, Ed Hoeffner, Carrie Wilmot.

PPX138 Poster Session I

Atomic Resolution X-ray Diffraction Studies of *E. coli* Dihydrofolate Reductase. Brad Bennett, Anna Gardberg, Elizabeth Howell, Chris Dealwis.

P139 Poster Session III

Structure of AICAR Transformylase in Complex with a Novel Inhibitor Identified *via* Virtual Ligand Screening. Lan Xu, Chenglong Li, Arthur Olson, Ian Wilson.

P140 Poster Session I

Novel Proteomics Research Information Management System (RIMS). M. Ruf, H. Thiele, B. Guigas.

P141 Poster Session I

Thermodynamic Studies of Ligand-binding and Conformational Changes of *B. stearrowthermophilus* Tryptophanyl-tRNA Synthetase (Trp-RS). Violetta A. Weinreb, Charlie W. Carter, Jr..

P142 Poster Session III

Deposition and Annotation at the RCSB PDB. Kyle Burkhardt, S. Dutta, Z. Feng, L.-C. Fernandez, V. Guranovic, S. Jain, R. Oughtred, I. Persikova, S. Richman, B. Schneider, Y. Yang, J. Yang, J. Westbrook, C. Zardecki, H. Berman.

P143 Poster Session III

PDB Depositions and Statistics from Synchrotron Sources. Jiansheng Jiang.

PP144 Poster Session I

Structural Bioinformatics of Protein-bound Water. Christopher A. Bottoms, Tommi White, John J. Tanner.

P145 Poster Session III

A Protein Family View of 3D Protein Structure Space Coverage. Dawei Lin, Zhou Yucho, Praissman Jeremy, Rose John, Wang Bi-Cheng.

P146 Poster Session III

A Generic Way to Combine Crystallographic Software. Jeremy Praissman, Dawei Lin, Zhi-jie Liu, Wolfram Tempel, John Rose, Bi-Cheng Wang.



## P147 Poster Session III

Galleries and Expanded Features of the NDB Atlas. Jasmin Yang, Joanna de la Cruz, Gregory Donahue, Zukang Feng, Bohdan Schneider, John Westbrook, Christine Zardecki, Helen M. Berman.

## PP148 Poster Session I

Structure-function Studies on the OhrR, Bacterial Transcription Regulator. Minsun Hong, John Helmann, Richard Brennan.

## P149 Poster Session II

A Comparison of Oct-1/DNA/SNAP190 Transcription Signaling Complexes. Stacy Hovde, Katherine Strong, Aimee Brooks, James Geiger.

## P150 Poster Session I

Unlocking the Secrets of Vitamin D-dependent Gene Regulation: Molecular Structures of Rat VDR-Ligand-coactivator Complexes. Janeen Vanhooke, Matthew Benning, Cary Bauer, Wesley Pike, Hector DeLuca.

## P151 Poster Session II

Structural Studies of SHOX-DNA Complex Involved in Growth Processes. Narendra Narayana.

## PX152 Poster Session I

Mapping and Crystallizing the Structural Domain of TAF4. Xiaoping Wang, Raymond H. Jacobson.

## P153 Poster Session II

Crystal Structure of YfiR, a Putative Transcriptional Regulator from *Bacillus subtilis*. Shyamala Rajan, Xiaojing Yang, Ludmilla Shuvalova, Frank Collart, Wayne Anderson.

## PP154 Poster Session I

The Interaction Between PurR and its Substrates. Jianghai Zhu, Alope Bera, Sangita Sinha, Howard Zalkin, Janet Smith.

## PP155 Poster Session II

The Crystal Structure of Rabbit Phosphoglucose Isomerase Complexed with an Analogue of the Open Chain Form of G6P, D-sorbitol-6-phosphate (S6P), at 2.0 Å Resolution. Ji Hyun Lee, Constance Jeffery.

## P156 Poster Session I

The Structure Determination of APC24466 from 1.4-Å SAD Data Collected at the Structural Biology Center 19BM Beamline. Rongguang Zhang, Frank J. Rotella, Ruiying Wu, Randy W. Alkire, Norma E.C. Duke, Andrzej Joachimiak.

## PP158 Poster Session I

Structure-based Engineering of Maltose Binding Protein. Patrick Telmer, Brian Shilton.

## PP159 Poster Session II

Time-resolved Crystallographic Studies of the Heme-based Sensor FixLH. Jason Key, Vukica Srajer, Reinhard Pahl, Keith Moffat.

## PP160 Poster Session I

Discovering the Mechanistic Pathway for HMG-CoA Reductase Using Time Resolved Laue Crystallography. Chandra Duncan, Calvin Steussy, Tim Schmidt, John Burgner II, Victor Rodwell, Cynthia Stauffacher.

## P161 Poster Session III

A Comparison of apo and Holoenzyme States of Phosphodiesterase 4D in Complex with (R)-Rolipram. Joseph Lomino, Alex Burgin, Robin Clark, Mark Gurney, Kathryn Hjerrild, Hidong Kim, Rama Mishra, Jasbir Singh, Lance Stewart, Bart Staker.

## PX162 Poster Session I

Structure of Aldose Reductase-inhibitor Complexes at Ultra-high Resolution from Helium Cooled Crystals. Stephan Ginell, T. Petrova, I. Hazemann, Alexandra Cousido, Andre Mitschler, F. Ruiz, M. Van Zandt, Andrzej Joachimiak, Alberto Podjarny.

## P163 Poster Session I

Success Rate Comparison of Sitting Drop Vapor Diffusion and Microfluidics Free-interface Diffusion Crystallization. Timothy Lekin, Brent Segelke.

## P164 Poster Session II

Optimizing Refined Molecular Fragments in a Cell. Douglas Powell.

## P165 Poster Session III

A Kit for the Construction of Three-dimensional Cartoon-style Models of Protein Structures. Richard Garratt, Leila Beltrami, Luciano Abel.

## P166 Poster Session I

XRPD Measurements on Single Crystal Diffractometers. Kingsley L. Smith, Scott K. Goodwin, R. Curtis Haltiwanger, Bob B. He.

## P167 Poster Session I

Crystal Structure of  $\text{Cd}_3(\text{O}_3\text{PC}_2\text{H}_4\text{CO}_2)_2 \cdot 2\text{H}_2\text{O}$ : Influence of the Solid State NMR in the Structure Determination. Abraham Clearfield, Naima Bestaoui, Xiang Ouyang, Florence Fredoueil, Bruno Bujoli.

## P168 Poster Session I

Adventures with Neutron Diffraction: Protonation States of D-xylose Isomerase. Gerard Bunick, B. Leif Hanson, Paul Langan, Amy Katz, H.L. Carrell, Benno Schoenborn, Jenny Glusker.

## P169 Poster Session I

Convergent Beam Neutron Crystallography. W. M. Gibson, J. M. Carpenter, H.H. Chen-Mayer, E.R. Maxey, D.F.R. Mildner, M.E. Miller, J.W. Richardson, A.J. Schultz, R. Youngman.

## P170 Poster Session I

Variable-temperature and Pressure Neutron-diffraction Studies of Short Strong N..H..O Hydrogen Bonds. John A. Cowan, Arthur J. Schultz.

## P171 Poster Session II

Crystal Structure and Charge Density Analysis of 1:1 Complex of 4-Nitrophenol and Ammonium 4-Nitrophenolate. Kenneth L. Martin, Madoka Hasegawa, Edwin D. Stevens.



- PP172 Poster Session I  
Charge Density Studies of Urotropine-N-oxide-formic Acid. Cara Nygren, Chick Wilson, John Turner.
- PP173 Poster Session II  
A Unique Heterotrimetallic  $\text{Cu}^{\text{II}}\text{Co}^{\text{III}}\text{Zn}^{\text{II}}$  Complex With Diethanolamine Ligand. Dmytro Nesterov, Valeriya Makhankova, Volodymyr Kokozay, Brian Skelton.
- PP174 Poster Session I  
Crystal Structure of a Novel Four-nuclear Heterometallic  $\text{Cu}^{\text{II}}/\text{Zn}^{\text{II}}$  Complex Obtained by Direct Template Synthesis. Denys Shevchenko, Svitlana Petrusenko, Vladimir Kokozay, Brian Skelton.
- P175 Poster Session II  
Three Polymorphs of Compound  $[\text{Mn}^{\text{II}}(15\text{-crown-5})(\text{H}_2\text{O})_2](\text{NO}_3)_2$ . Xiang Hao, Sean Parkin, Carolyn Brock.
- P176 Poster Session I  
Systematics of Non-merohedral Twinning of Chiral Aziridines. Maren Pink.
- PPX177 Poster Session I  
Copper(II) Complexes with Schiff's Basis: Characterization and Crystallographic Structure. Érica Tozzo, Regina Santos, Maria Gambardella, Mirian Santos, Sandra Romera, Edward Dockal.
- P178 Poster Session II  
On Desymmetrization and Relativistic Contraction in 4d Atoms. Boris Udovic.
- P179 Poster Session II  
Molecular Structure of Hydrazide-containing Copper(III) Macrocyclic Complexes Obtained by Template Synthesis. Olga Kanderl, Igor Fritsky, Roland Kramer, Alexandra Cosma, Hans Pritzkow.
- PP180 Poster Session I  
In Search of the Structural Determinants of Optical Activity. Kacey Claborn, Werner Kaminsky, Bart Kahr.
- P181 Poster Session II  
Structure Details of Polymorphism in Organic Light Emitting Diode, OLED, Material, Alq<sub>3</sub>. Manju Rajeswaran, Thomas Blanton.
- PPX182 Poster Session II  
Polymorphism, Hydration and Metal - Metal Contacts in a Luminescent Platinum Dicarbene. Jay Stork, Marilyn Olmstead, Alan Balch.
- P183 Poster Session II  
Combined Synchrotron Powder Diffraction and Solid-state NMR Studies of Ambucic Acid. James Harper, Yuegang Zhang, Peter Lee, Robert Von Dreele, David Grant.
- P184 Poster Session II  
Rapid Charge Density Data Collection. Damon Parrish, J. Deschamps, A. Coop, L. Thatcher, H. Wu, J. Ferrara, L. Daniels.
- P185 Poster Session III  
Performance Characteristics of a New Confocal MaxFlux Optic Coupled with a Sealed Tube Source. Kris Tesh, Angela Criswell, Adam Courville, Bret Simpson, Eric Hnath, Joseph Ferrara, Boris Verman, Licai Jiang.
- P186 Poster Session III  
Structural Investigations of Microcrystalline Cellulose-drug Systems. S.A. Fasilova, N.D. Burkhanova, S.M. Yugay, G.V. Nikonovich, S.Sh. Rashidova.
- P187 Poster Session I  
Advances in Instrumentation for Automated Combinatorial Crystallization Screening. Brent Segelke, Timothy Lekin, Dominique Toppani, Mary Cornett, Jim Johnson, David Martin.
- P188 Poster Session III  
Fully Automated Workstation for Vapor Diffusion and Microbatch Protein Crystallography. Kirby Reed, Niki Popp, Joan Stevens.
- P189 Poster Session I  
Structural Characterization of the Closed Conformation of Mouse Guanylate Kinase. Nikolina Sekulic, Ludmilla Shulvalova, Arnon Lavie.
- P190 Poster Session III  
Evaluating and Determining Precision and Accuracy for Nanoliter Volumes of Viscous Solutions on an Automated Liquid Handling Instrument. Niki Popp, Tim Hegeman, Joan Stevens, Kirby Reed.
- PP191 Poster Session I  
Approximating Short-range Lee-Richards Molecular Surfaces by Blurring. Peter Zhivkov, Herbert Bernstein.
- PP192 Poster Session II  
On Forced Reflection New Application in the Area of X-ray Diffraction. Marut Navasardyan.
- P193 Poster Session III  
Crystal Structure of a Homolog of the RNase P Protein Rpp29 from the Archaeon *Archaeoglobus fulgidus*. David Sidote, David Hoffman.
- PPX194 Poster Session I  
Arginine Decarboxylase a Target for the Design of Novel Bio-defense Agents against Plague: Structural Investigation. Chandra Patel, Robert Adcock, Marcos Oliveira.
- P195 Poster Session III  
Crystallographic and Kinetic Studies of Novel SARS-CoV 3CLpro Protease Inhibitors that Inhibit SARS-CoV and MHV-A59 Replication. Andrew Mesecar, K. Ratia, B. Santarsiero, K. Xi, D. Jukneliene, B. Harcourt, P. Rota, S. Baker, A. Ghosh, W. Fu, M. Johnson.
- PP196 Poster Session I  
Crystal Structure of HI0607 Identifies a Novel Shikimate Dehydrogenase from *Haemophilus Influenzae*. Sasha Singh, S. Korolev, O. Koroleva, T. Zarebinski, F. Collart, A. Joachimiak, D. Christendat.



P197 Poster Session III

Ninety-six (96) Crystallization Optimization Conditions in Less than 10 minutes Using a New Pre-filled Microplate. Steve Tetreault, Christian Houde.

P198 Poster Session II

Cyclic Voltammetry Influence on the Crystallization Process of Ferritin for Atomic Force Microscopy and X-ray Diffraction. Margarita Rivera, Abel Moreno.

P199 Poster Session III

Ten Years of CCD Detectors. R. Curtis Haltiwanger, Charles F. Campana, Michael Ruf, Timothy Thorson.

PPX200 Poster Session I

Crystal Structure of *E. coli* Dihydrofolate Reductase Bound to a Novel Potent Inhibitor. Rachael Summerfield, Murray Junop.

P201 Poster Session III

HPC and Grid Applications in High Throughput Protein Crystallography. Ronan Keegan, Dave Meredith, Graeme Winter, Martyn Winn.

P202 Poster Session III

SAXS of Lens Crystallin Proteins. Amir Mirarefi, S. Boutet, A. Kiss, A. DeVries, C. Cheng, I.K. Robinson, C. Zukoski.

P203 Poster Session III

Viscosity of the Solution is Crucial for the Protein Crystallization to Enhance the Effects of Microgravity Environment. Hiroaki Tanaka, Koji Inaka, Shigeru Sugiyama, Sachiko Takahashi, Satoshi Sano, Masaru Sato, Susumu Yoshitomi.

P204 Poster Session III

A Simplified and High-density Counter-diffusion Method for a Protein Crystallization. Masaru Sato, Hiroaki Tanaka, Koji Inaka, Shigeru Sugiyama, Sachiko Takahashi, Satoshi Sano, Susumu Yoshitomi.

PP205 Poster Session I

Phase Behavior and Structure of  $C_8\beta G_1/C_8E_3$  Surfactant Solutions and their Role in Membrane Protein Crystallization. Gabriella Santonicola, Eric Kaler, Abraham Lenhoff.

P206 Poster Session III

Designing More Efficient Crystallization Screening Experiments: Consider Protein Isoelectric Point. K.A. Kantardjiev, B. Rupp.

P207 Poster Session III

Optimal Data Collection Strategies for SAD Datasets in the Home Laboratory. Cary Bauer, Matthew Benning, Michael Ruf, Joerg Kaercher.

P208 Poster Session III

Automated Sample Screening and Data Collection Using BruNo. Matthew Benning, Joerg Kaercher, Robert Lancaster, Steven Leo, Frank Jin.

P209 Poster Session III

CMCF08ID-1 Beamline at the Canadian Light Source. Pawel Grochulski, Riccardo Signorato, Ingvar Blomqvist, Louis Delbaere.

P210 Poster Session III

FASTSHUT: Flash-annealing of Cryo-protected Samples. Jean Jakoncic, A. Lenhard, Z. Lin, C. Barret, A. Vahedi-Faridi, V. Stojanoff.

P212 Poster Session III

Wide Angle X-ray Solution Scattering as a Probe of Ligand-Induced Conformational Changes in Proteins. Robert Fischetti, Diane Rodi, David Gore, Lee Makowski.

P213 Poster Session III

Development of the Cryoprotectant Database for Protein Crystallization Experiments and its Statistics. Sachiko Takahashi, Takashi Yoshimine, Masaru Sato, Hiroaki Tanaka, Kensaku Hamada, Susumu Yoshitomi.

P214 Poster Session III

Progress in the Robotic Sample Changer System Development for the SBC-CAT. Deming Shu, C. Preissner, D. Nocher, Y. Han, P.W-K Lee, S. Ginell, R. Alkire, K. Lazarski, R. Schuessler, A. Joachimiak.

P215 Poster Session III

Hydride-induced Lattice Strains in Epitaxial Niobium. Brent Heuser, Monica Allain.

P216 Poster Session III

The Local Atomic Structure of Nanocrystalline K-Li-Mn-O-I Studied with Pair Distribution Function Analysis. Milen Gateshki, Seong-Ju Hwang, Valeri Petkov, Gabriel Ghita.

P217 Poster Session I

Phase Transformations in Rare Earth Titanates. Waltraud Kriven, Kerstin Jurkschat.

P218 Poster Session III

Diffraction Studies of  $NaAlH_4$  Doped with Ti. Claudia Rawn, Joachim Schneibel, Scott Speakman, Jane Howe, Bryan Chakoumakos, Lachlan Cranswick, Ian Swainson.

P219 Poster Session III

Topological Relaxation of a Shear-induced Lamellar Phase to Sponge Equilibrium and the Energetics of Membrane Fusion. William Hamilton, Lionel Porcar, Paul Butler, Gregory Warr.

P220 Poster Session III

SAXS Study of Protein-polymer Interaction. Iris Torriani, Cristiano Oliveira, Nara Almeida, Watson Loh.

P221 Poster Session III

Multi-component Characterization of Commercial Ceramics and Metal Alloys by Anomalous USAXS. Pete R. Jemian, Gabrielle G. Long, Rosario A. Gerhardt, Sheldon M. Wiederhorn, Frantisek Lofaj, Jan Ilavsky.

PP222 Poster Session II

Are We Compatible For Each Other...What if Hydrogen Bonds Could Talk? Nate Schultheiss, Christer Aakeröy, John Desper.



PP223 Poster Session II

Amide-amide Hydrogen Bonds and Flexible Ligands as Linkers for Deliberate Supramolecular Inorganic-organic Frameworks. Joaquin Urbina, Christer Aakeröy, John Desper.

PP224 Poster Session II

N-substituted Pyrazoles - LEGO for Chemists? Benjamin Scott, Christer Aakeröy, John Desper.

PP225 Poster Session II

Supramolecular Reagents for One-pot Assembly of Quaternary Molecular Architectures. Debra Salmon, Christer Aakeröy, John Desper.

PP226 Poster Session II

Supermolecules a Quarte. Brock Levin, Christer Aakeröy, John Desper.

P227 Poster Session II

Lattice Interpenetration and Other Adventures in Network Solids with NC-M-CN Rungs (M = Ag, N). Urs Geiser, John A. Schlueter.

PPX228 Poster Session II

If There was a Fourth Little Pig He Would Have Built His House Out of These.... Michelle Smith, Christer Aakeröy, John Desper.

P229 Poster Session II

Polymorphism in Tris (5-acetyl-3-thienyl) Methane (TATM) Inclusion Compounds with 1,3-dichloropropane Guest. Gary Enright, Paul Sidhu, John Ripmeester.

P230 Poster Session II

Crystallographic and Theoretical Studies on the Role of Halogen-halide Synthons in the Structures of (nYP)X, (nYP)<sub>2</sub>CuX<sub>4</sub> and Cu(nYP)<sub>2</sub>X<sub>2</sub>. Firas Awwadi, Roger Willett, Kirk Peterson, Brendan Twamley.

PPX231 Poster Session II

Low Temperature Investigation of Gas Molecules in a Porous Metal-organic Framework. Jesse L.C. Rowsell, Elinor C. Spencer, Garry J. McIntyre, Juergen Eckert, Judith A.K. Howard, Omar M. Yaghi.

PPX232 Poster Session II

Structure of Supramolecular Synthons Based on Propargylic Alcohol Derivatives. Marilise A. Hyacinth, Michal Sabat, Ge Gao, Lin Pu.

PPX233 Poster Session II

Self-assemble of Hydrogen-bonding and Pi-stacking Polymers for Transitions Metals Complexes. Janaina Ferreira, Regina Santos, Adelino Neto, Mauro Eduardo.

PPX234 Poster Session II

Polar Ordering and Electric Field-induced Domain Reorientation in Channel Inclusion Compounds. Jeremy Rush, Mark Hollingsworth, Mark Abel.

P235 Poster Session II

Ferrocenylbenzoyl thienyl/thiazolyl Esters. John F. Gallagher, Steven A. Alley, Vincent M. Hooper, Peter T.M. Kenny, Alan J. Lough.

P236 Poster Session I

The Structural Biology Center User Program at the Advanced Photon Source, Argonne National Laboratory. Stephan L. Ginell, Randy Alkire, Marianne Cuff, Norma E.C. Duke, Youngchang Kim, Krzysztof Lazarski, Jerzy Osipiuk, Frank Rotella, Rongguang Zhang, Andrzej Joachimiak.

P237 Poster Session I

Cold Neutrons for Biology and Technology. Stephen White, Joseph Dura, Charles Majkrzak, Mathias Loesche, Susan Krueger.

P238 Poster Session I

The PCS Facility for Neutron Protein Crystallography at Los Alamos. Benno P. Schoenborn, Paul Langan.

P239 Poster Session I

GM/CA: A New NIH-funded Sector for Protein Crystallography at the APS will Provide Two Independent Undulator Beamlines. Ward Smith, R.F. Fischetti, J.L. Smith, R. Benn, S. Stepanov, S. Xu, A. Urakhchin, O. Makarov, R. Sanishvili.

P240 Poster Session I

Design of a Single Crystal Macromolecular Neutron Diffractometer at the SNS. A.J. Schultz, P. Thiyagarajan, C. Rehm, J. P. Hodges, W.T. Lee, A.D. Mesecar, D.A. Myles, P.A. Langan.

P241 Poster Session I

New SANS Instrumentation at Oak Ridge National Laboratory. G. W. Lynn, M.V. Buchanan, P.D. Butler, W.T. Heller, D.A.A. Myles, V.S. Urban, G.D. Wignall.

P242 Poster Session I

The Center for Structural Molecular Biology at Oak Ridge National Laboratory. Volker Urban, William Heller, Gary Lynn, Paul Butler, George Wignall, Michelle Buchanan, Dean Myles.

P243 Poster Session I

The HFIR Center for Neutron Scattering. B. Chakoumakos.

P244 Poster Session I

Northeastern Collaborative Access Team Beam Lines at the Advanced Photon Source. Steven E. Ealick, Malcolm Capel, Kazimierz Gofron, Igor Kourinov, Christopher Lehmann, Ed Lynch, Craig Ogata, Narayanasami Sukumar, Jun Wang, James Withrow.

P245 Poster Session I

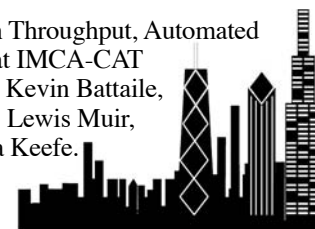
MacCHESS: A World-class Facility for Crystallography at Cornell. David Schuller, M. Cook, U. Englich, R. Gillilan, Q. Hao, C. Heaton, I. Kriksunov, W. Miller, D. Szebenyi.

P246 Poster Session I

Microcrystal Small Molecule X-ray Crystallography at the Advanced Light Source. Allen Oliver, Simon Clark, Sirine Fakra, Frederick Hollander, Howard Padmore, Al Thompson.

P247 Poster Session I

Integration of Robotics for High Throughput, Automated Screening and Data Collection at IMCA-CAT at the Advanced Photon Source. Kevin Battaile, Anne Mulichak, Irina Koshelev, Lewis Muir, Katie Favale, Ann Bertling, Lisa Keefe.



P248 Poster Session I

“He who Scatters has Much”: Neutron Powder Diffraction Facilities at the NRC, Chalk River, Canada. Lachlan Cranswick, Ian Swainson.

P249 Poster Session I

SMART Teams: Students Modeling a Research Topic. J. Morris, S. Coltn, M. Patrick, T. Herman.

P250 Poster Session I

Integration of PDB Resources and SMART Teams into the High School Curriculum. Tommie S. Hata.

P251 Poster Session I

Water Water Everywhere: How Aquaporin Works. Nathan Theobald, Ashley Bray, Rebecca Denison, Martie Dowis, Simon Schmidt, Tony Schuler, Tisha Williams, Pete Nielson, Karen DeBoer.

P252 Poster Session I

The Structure and Function of Myelin Oligodendrocyte Glycoprotein-MOG. Katy Keefe, Cristina O’Brian, Hannah Gottinger, Alyssa Latin-Kasper, Megan McChair, Jeff Anderson.

P253 Poster Session I

Hemophilia A, A Bleeding Disorder Involving Coagulation Factor VIII. Beneva Myrick, Mike Piotrowski, Maixiong Thao, Yangyee Tyhao, Dean Dolenece.

P254 Poster Session I

Mammalian Cytochrome P450. A. Amasino, W. Baatacharya, E Betlach, H. Cronan, Y. Deng, S. Huang, B. Jackson, O. Judd, I. Lee, Y. Pu, H. Streckert, P. Vander velden, G. Graper.

P255 Poster Session I

The  $\alpha$ -V- $\beta$ -3 Integrin Molecule. K. Brenner, D. Brown, S. Flaaten, T. Grewal, L. Hirschmann, L. Moon, M. Roberts, L. Stewart.

P256 Poster Session I

GCN5, A Key to Opening DNA. K. Bauer, A. Benz, B. Berg, L. Breu, B. Brophy, M. Dougherty, A. Limbach, M. Masterson, D. Miller, K. Moakley, T. Meuller, D. Polaski, A. Puzach, D. Rayburn, M. Ruka, A. Solberg, L. Spaits, D. Tighe, B. Tushaus, K. Volbrecht, R. Widmann, D. LaFlamme.

P257 Poster Session I

Splicesomes are as Essential to Life as Breathing: U1A, a Component of Spliceosomes. Jessica Jacob, Danielle Mattson, Rebecca Easter, Bai Yang, Megan Kaiser, Shari Gajria.

P258 Poster Session III

Automated Applications of BnP.II. Test Results. Charles M. Weeks, S.A. Potter, H. Xu, R. Miller, L. Pasupulati, W. Furey.

P259 Poster Session II

A Microfluidic System for Screening Protein Crystallization Conditions inside Nanoliter Droplets with On-chip X-ray Diffraction. Bo Zhengrustem Rustem Ismagilov, L. Spencer, Roach, Josh Tice, Cory J. Gerdts, Delai Chen.

P260 Poster Session III

A Simple Method for the Identification of Protein/Ligand Complexes Using Protein Powder Diffraction. Marc Allaire, Natalia Moiseeva, Cristian Botez, Peter Stephens.

P261 Poster Session II

Structural Mechanism for T7 RNA Polymerase Translocation. Whitney Yin.

PX262 Poster Session II

Structural Studies of the SV5 Hemagglutinin-Neuaminidase (HN) Tetramer. Ping Yuan, Tom Thompson, Reay G. Paterson, Robert A. Lamb, Theodore Jardetzky.

P263 Poster Session II

Structural Studies of *E. coli* Transhydrogenase A Multi-technique Approach for Membrane Proteins. Holly Heaslet, Musto Yamaguchi, Vidyasankar Sundaresan, Mark Yeager, C. David Stout.

PPX264 Poster Session II

The Real Modulated NdTe<sub>3</sub> Structure Type and its Properties: A Combined Superspace Group/Pair Distribution Function Analysis Approach. Christos Malliakas, HyunJeong Kim, Daniel Bilc, Simon Billinge, Bhanu Mahanti, Mercouri G. Kanatzidis.

P265 Poster Session III

High-energy Resonant Scattering Studies of the Pb/Bi Distribution in the Thermoelectric Material Pb<sub>5</sub>Bi<sub>6</sub>Se<sub>14</sub>. Yuegang Zhang, Sarvjit D. Shastri, Deming Shu, Peter L. Lee, Duck-Young Chung, Mercouri G. Kanatzidis, Angus P. Wilkinson.

P266 Poster Session III

X-ray Microbeam Diffraction for Protein Crystallography Using FZP. Keiko Miura Akihisa Takeuchi Hidekazu Takano Kentaro Uesugi Nobuhisa Shimizu Yoshio Suzuki

P267 Poster Session III

Studies of Antibiotic Resistance in *S. pneumoniae*. Lucile Pernot, Laurent Chesnel, Audrey Le Gouellec, Jacques Croize, Thierry Vernet, Andre Zapun, Andrea Dessen, Otto Dideberg.

PP268 Poster Session II

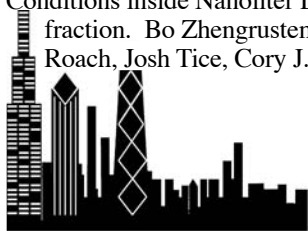
Structure of the Thiazole Synthase/ThiS Complex, an Essential Component of Thiamin Biosynthesis in *Bacillus subtilis*. Ethan Settembre, Pieter Dorrestein, Huili Zhai, Abhishek Chatterjee, Fred McLafferty, Tadhg Begley, Steven Ealick.

P269 Poster Session III

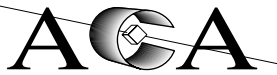
Why Does TNA Cross-Pair More Strongly with RNA Than with DNA? - An Answer From X-ray Analysis. Pradeep S. Pallan, Albert Eschenmoser, Christopher J. Wilds, Zdzislaw Wawrzak, R. Krishnamurthy, Martin Egli.

PPX270 Poster Session II

Domain Organization of *Salmonella typhimurium* Formylglycinamide Ribonucleotide Amidotransferase Revealed by X-ray Crystallography. Ruchi Anand, Steve Ealick, Joanne Stubbe, Aaron Hoskins.







# REGISTRATION FORM

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**\*Increment charged to non-member registration may be credited toward new member dues for 2004 by submitting a membership application form with the registration form.**

All prices are listed in U.S. dollars and must be submitted in U.S. dollars. Purchase orders will not be accepted. Only U.S. checks, VISA, MasterCard and American Express payments will be accepted. ACA, E.I.N. 22-6075182.

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**Mail or fax this form by July 2.  
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Are you an invited speaker? If yes, list session number \_\_\_\_\_

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## WORKSHOPS

Registration for workshops WK.01, WK.02, WK.04, WK.05, only available to U.S. citizens before June 25 due to visitor clearance restrictions. The time limitation for clearance for non U.S. citizens is past.

- |   |   |
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| <input type="checkbox"/> <b>WK01</b> : MAD/SAD<br>Students-\$140 Others-\$160 | <input type="checkbox"/> <b>WK04</b> : GM/CA- Synchrotrons<br>Students-\$60 Others \$80 |
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## SOCIAL PROGRAM

### Opening Reception - Saturday, July 17

- No Fee for Registered Participants**  Will Attend  Won't Attend  
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### YSSIG Mentor/Mentee Dinner - Sunday, July 18

- Mentee \$10 ticket # of tickets \_\_\_\_\_  
 Mentor \$10 ticket # of tickets \_\_\_\_\_

### YSSIG Mixer - Monday, July 19

- No Fee for Registered Students, Postdocs, Young Scientists**  
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**All others \$10**  # of tickets \_\_\_\_\_

### Awards Banquet - Wednesday, July 21

- \$55 ticket # of tickets \_\_\_\_\_  
 \$25 student ticket # of tickets \_\_\_\_\_

#### Entree choice:

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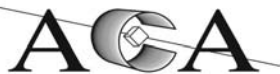
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