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WK.01 Magnetic Structure Analysis by Neutron Diffraction TechniquesO. Garlea, *301A*
B. Chakoumakos, Presiding

08:00-08:30 Introduction. O. Garlea, ORNL.

08:30-09:45 Introduction to Magnetic Diffraction. Application of Group Theory to Magnetic Structure Determination. A.S. Wills, Univ. College London.

10:00-11:00 Spherical Neutron Polarimetry in Magnetic Structure Determination. E. Ressouche, CEA.

11:00 - 12:00 Polarized Neutron Study of the Magnetization Density Distribution. The Flipping Ratio Method. A. Gukasov, CEA Saclay.

12:00-01:00 Lunch Break (provided).

01:00-02:30 Recent Developments in Refinement Techniques. Simulated Annealing Algorithm with FULLPROF. J. Rodriguez-Carvajal, ILL.

02:30-03:00 Coffee Break.

03:00-06:30 Hand-on Session: Exercises. O. Garlea, A. Moreira Dos Santos, B. Chakoumakos.

WK.02 Neutron Macromolecular Crystallography from Expression to RefinementLeighton Coates, *301B*
Paul Langan, Presiding

08:25-08:30 Welcome. Leighton Coates, ORNL.

08:30-09:15 Introduction and Protein Perdeuteration. Kevin Weiss, ORNL.

09:15-09:50 Optimal Protein Crystallization Techniques. Nobuo Niimura, Ibaraki.

09:50-10:30 Hydrogen Deuterium Exchange Patterns. Chris Dealwis, Case Western.

10:30-11:00 Coffee Break.

11:00-11:30 Structural Highlight-Joint Refinement of DFPase. Julian Chen, Frankfurt.

11:30-12:00 New Neutron Beamlines. Christina Hoffman, ORNL.

12:00-12:30 LADI III and D Lab. Mathew Blakeley, ILL

12:30-01:30 Lunch Break.

01:30-1:35 Tutorial Overview. Paul Langan, LANL.

01:35-03:00 nCNS. Marat Mustyaki-mov, LANL.

03:00-03:30 Coffee Break.

03:30-05:00 phenix.refine. Pavel Afonine, LBNL.

WK.03 Wise Use of Dose: Structure Solvability vs. Structure IntegrityGerd Rosenbaum, *301C*
Zbigniew Dauter, Presiding

08:00-08:10 Welcome and Introduction. Gerd Rosenbaum.

08:10-08:40 Radiation Damage in Macromolecular Crystallography: What is it and Why Do We Care? Elspeth Garman.

Topic 1: How Much Exposure is Enough?

08:40-09:05 How Much Exposure is Enough for Anomalous Phasing and Refining a Structure at Different Resolutions? Zbigniew Dauter, Gerd Rosenbaum.

Topic 2: Techniques to Reduce Overall Dose for Same Final Structure Solving Result

09:05-09:30 BEST - A Program for Optimal Data Collection Strategy. Alexander Popov.

09:30-10:00 Coffee Break.

10:00-10:30 Panel Discussion on Benefits of (a) Orienting Crystal for Bijvoet Pairs on Same Frame and of (b) Re-orienting Crystal During Data Collection over Rotation Angle Larger than Required by Symmetry vs. No Change of Orientation. Panel Members: Zbyszek Otwinowski, Zbigniew Dauter, TBA.

10:30-10:55 A Multiple-Data-Set 2 Data Collection Strategy for a Better Data Set Within a Fixed X-ray Dose. B.C. Wang.

10:55-11:20 Limit of Multiple Data Set Strategy? Does Longer Exposure Time at Same Dose Help? Zbigniew Dauter, Gerd Rosenbaum.

11:20 - 11:35 Is the Multiple Data Set Strategy Valid for Photon Counting Detectors? Vincent Olieric.

Topic 3: Mitigation of Radiation Damage

11:35-12:00 Scavengers - Do They Help? Role of Cryoprotectant. Elspeth Garman.

12:00-01:00 Lunch Break.

01:00-01:30 Low Temperature - Decrease of Damage in General of Site-Specific Damage Only? Speaker TBA.

01:30-01:50 Computational - Intelligent Extraction of Small Signals. Zbyszek Otwinowski.

01:50 - 02:15 RADDOSE - Be Aware of What Your Solvent Adds to the Dose. Elspeth Garman.

Topic 4: Reduction of Background Noise for Better I/σ(I)

02:15-02:40 Optics and Sample Induced Background vs. Scattering Angle. Randy Alkire.

02:40-03:10 Coffee Break.

03:10 - 03:35 Detector Distance - Beam Spot Size and Sample Induced Spot Size vs. Mosaicity and Scattering Angle. Zbigniew Dauter, Gerd Rosenbaum.

03:35-04:00 Detector Induced Noise - Advantage of Photon Counting Detector Pilatus 6M over analog CCD detectors. Vincent Olieric.

Topic 5: Optimal Choice of Wavelength

04:00-04:25 Radiation Damage For Same Statistical Significance of Measured Diffraction Intensities vs. Absorbed Dose at Different Wavelength - A Few Observations - But No Systematic Study To Date. Gerd Rosenbaum.

Topic 6: Minibeams

04:25-04:50 Reduced Absorbed Dose With Micrometer Size Beams Robert Fischetti, Ruslan Sanishvili.

04:50-05:20 Take Home Lesson Panel Discussion. Moderator Zbigniew Dauter.

WK.04 Structural Biology without Crystals: Small-Angle Scattering Methods

Susan Krueger, Volker Urban, Presiding *301D*

08:30-08:45 Welcome and Introduction.

08:45-09:30 Introduction to Small-Angle Scattering (SAS). P. Thiyagarajan, ANL.

09:30-10:15 Correct Use of Modeling Software for SAS Data. Dmitri Svergun, EMBL

10:15-10:45 Coffee Break.

10:45-11:30 Labeling and Contrast Variation. Susan Krueger, NIST & Kevin Weiss, ORNL.

11:30 -12:00 Recent Advances in Time-Resolved SAS. Theyencheri Narayanan, ESRF.

12:00-12:30 State-of-the-Art Grazing Incidence SAS. Byeongdu Lee, APS.

12:30-2:00 Lunch Break.

02:00-02:45 Introduction to Reflectometry. Chuck Majkrzak, NIST.

02:45 -03:30 Correct Use of Modeling Software for Reflectometry Data. Paul Kienzle, UMD/NIST.

03:30-04:00 Coffee Break.

04:00-04:30 Phase-Inversion Neutron Reflectometry Methods. Ursula Perez-Salas, ANL.

04:30-05:00 Recent Advances in Reflectometry Techniques for Studying Membrane Proteins. Frank Heinrich, CMU/NIST.

05:00-05:30 Discussion and Wrap Up: What are the Next Horizons for Neutron and X-ray Scattering in Biology?

2008 Margaret C. Etter Student Lecturer Awards

Each Special Interest Group (SIG) within the ACA has the opportunity to select one student to receive an award and to present a lecture in one of the sessions organized by that SIG. Selections are based upon submitted abstracts and are independent of whether the student presenter originally requested an oral or poster presentation. Award winners are determined by the elected officers of the SIGs. Students who are selected will receive a monetary award of \$250 and a certificate.

Congratulations to this year's winners:

Biological Macromolecules	Alexey Amunts, Tel Aviv University, Isreal	01.03.05
Fiber Diffraction	Olga Antipova, Illinois Institute of Technology	02.01.06
Neutron Scattering	Matthew Hudson, Syracuse University	06.01.06
Small Angle Scattering	Karen Mulfort, Northwestern University	13.08.06
Small Molecules	Clare Yannette, Georgetown University	13.10.06
Synchrotron Radiation	Sterling Cornaby, Cornell University	13.14.03
Materials Science	Xuerong Liu, University of California, San Diego.....	13.15.05
Powder Diffraction	Daniel Mitchell, University of Tennessee.....	13.15.06
Young Scientist.....	Aruna Shankaranarayanan, University of Michigan	AW.01.05

SUNDAY, JUNE 1

Registration Desk07:30am-05:30pm.....Herley Concourse
 Speaker Ready Room07:30am-05:30pm.....301A
 Council Meeting Room.....07:30am-05:30pm.....Rontunda

Opening Ceremony08:00am-08:30am.....Ballroom C
 Exhibit Show10:00am- 04:30pm.....Exhibit Hall B
 Rigaku Luncheon12:00PM
 Poster Session I04:30pm-06:30pm.....Exhibit Hall B
 Tour to Oak Ridge Lab06:00pm busses begin loading

Opening Ceremony and Welcome**08:00am Ballroom C****Marvin Hackert, ACA President, Presiding****01.01 New Structures**

David Giedroc, Ballroom C
Mark Wilson, Presiding

08:30-09:00 01.01.01
 4-Amino-5-hydroxymethyl-2-methyl-
 pyrimidine Phosphate Synthase is a Novel
 Member of the Radical SAM Superfamily.
 Steve Ealick.

09:00-09:30 01.01.02
 Capturing Hammerhead Ribozyme Struc-
 tures in Action by Altering the Rate of Ca-
 talysis. Young-In Chi, Monika Matrick, Ro-
 salind Kim, William Scott, Sung-Hou Kim.

09:30-10:00 01.01.03
 Activation of the Interferon Regulatory Fac-
 tors: Crystal Structure of Dimeric IRF-5.
 William Royer, Weijun Chen, Suvana Lam,
 Hema Srinath, Celia Schiffer, Kai Lin.

10:00-10:30 Coffee Break.

10:30-11:00 01.01.04
 Structure and Mechanism of a Metal Sens-
 ing Regulatory RNA. Arati Ramesh, Cath-
 erine Wakeman, Charles Dann, Wade Win-
 kler.

11:00-11:30 01.01.05
 Structure Determination of a Substrate-
 channeling Proline Catabolic Enzyme using
 Deviant Crystals. Jack Tanner.

11:30-12:00 01.01.06
 Structural Mimicry and Ribosome Manip-
 ulation by a Viral RNA. Jeffrey Kieft, Da-
 vid Costantino, Jennifer Pflingsten, Amanda
 Keel.

06.01 Structure and Dynamics of Hydrogen Bonded Systems

Bruce Hudson, 301DE
Tom Koetzle, Presiding

08:25-08:30 Introduction.

08:30-09:00 06.01.01
 Neutron Diffraction Studies of Hydrogen
 Bonded Systems: An Overview. Thomas F.
 Koetzle.

09:00-09:30 06.01.02
 Complementary Single-crystal X-ray
 Diffraction and Neutron Powder-diffraction
 Studies of Hydrogen-bonded Small-
 molecule Systems at High Pressure. D.R.
 Allan.

09:30-10:00 06.01.03

Solid-state NMR and the Strong Hydrogen
 Bond. Gerard S. Harbison, Jun Zhou,
 Xingang Zhao.

10:00-10:30 Coffee Break.

10:30-11:00 06.01.04
 Quantum Wavepacket *ab initio* Molecular
 Dynamics: An Approach for Computing
 Dynamically Averaged Vibrational Prop-
 erties Including Critical Nuclear Quantum
 Effects. Srinivasan Iyengar.

11:00-11:30 06.01.05
 Deep Inelastic Neutron Scattering
 Measurements of Born-Oppenheimer
 Potentials and the Dynamics of Hydrogen
 Bonds. George Reiter.

11:30-11:45 06.01.06
 Single Crystal Neutron Diffraction and
 Inelastic Neutron Scattering Spectroscopy
 of Proton Conductor Lithium Hydrazinium
 Sulfate. Matthew Hudson, Paula M.B.
 Piccoli, Arthur J. Schultz, Bruce S. Hudson.

11:45-12:00 06.01.07
 Neutron Diffraction Structure of a Discrete
 Dichloride Hexahydrate Cube as a Tris(diis-
 opropylamino)cyclopropenium Salt. Paula
 Piccoli, Arthur Schultz, Owen Curnow,
 James Butchard, David Garrett, Robert
 Maclagan.

12:00-12:05 Concluding remarks.

09.01 Understanding the Nano-scale Using Small Angle Scattering

Greg Beaucauge, 301B
Ken Littrell, Presiding

08:30-09:00 09.01.01
 Dynamics and Thermodynamics at
 the Nanoscale. Michael Mackay, Erin
 McGarrity, Phillip Duxbury, Amalie Frisch-
 knecht, Anish Tuteja, R.S. Krishnan, Jon
 Kiel, Jon Seppala, Erica Tseng.

09:00-09:30 09.01.02
 New Insight into Hierarchical Structures
 of Carbon Black Dispersed in Polymer
 Matrices: A Combined Small-angle Scat-
 tering Study. Tadanori Koga, Takeji
 Hashimoto, Mikihiro Takenaka, Kazuya
 Aizawa, Naoya Amino, Masao Nakamura.

09:30-10:00 09.01.03
 Composite Polymer-nanoparticles Aggre-
 gates in Mixed Complex Systems Seen by
 Small Angle Neutron Scattering. Franaois
 Boue, Fabrice Cousin, Jeremie Gummel,
 Chloe Chevigny, Nicolas Jouault, Sophie
 Lorrain, Sebastien Alexandre, Gwanall
 Bourget, Jacques Jestin.

10:00-10:30 Coffee Break.

10:30-11:00 09.01.04
 Nanoscale Structure and Dynamics of
 Self-assembling Soft Matter Probed
 by Synchrotron SAXS. Theyencheri
 Narayanan, Drazen Zanchi, Anuj Shukla,
 Thomas Weiss, Michael Gradzielski.

11:00-11:30 09.01.05
 SANS and SAXS Characterization of
 Block Copolymer/Bioinspired Mineral
 Nanocomposite Gels. Pappannan Thiya-
 garajan, Umai Kanapathipillai, Surya
 Mallapragada.

11:30-11:50 09.01.06
 Characterization of Proteins Entrapped
 in Sol-Gel Materials using Small Angle
 Neutron Scattering. Hugh O'Neill, Guang-
 ming Luo, Volker Urban, Qiu Zhang, Del
 Castillo Alexis Rae.

11:50-12:10 09.01.07
 Understanding Shear Induced Collapse of
 Entropically Stabilized Lamellar Phases.
 Paul Butler, Vera Stoppelkamp, Lionel
 Porcar, William Hamilton.

13.01 Incommensurate and Modulated Structures

Lee Daniels, Presiding 301C

08:25-08:25 Welcome and Introduc-
 tion. Lee Daniels.

08:25-08:50 13.01.01
 Introduction to Modulated Structures. Lee
 Daniels, Christer Svensson.

08:50-09:15 13.01.02
 Crystallographic Computing System
 Jana2006. Michal Dusek, Vaclav Petricek,
 Lukas Palatinus.

09:15-09:40 13.01.03
 New Software Tools for Indexing and
 Processing of Modulated Structures.
 Michael Ruf, Marilyn Olmstead, Trixie
 Wagner, Andreas Schönleber.

09:40-10:05 13.01.04
Generating and Visualizing One-dimensional Incommensurate Structural Modulations. Branton J. Campbell, Harold T. Stokes.

10:05-10:30 Coffee Break.

10:30-10:55 13.01.05
There and Back Again: A Crystallographer's Tale of Modulated Protein Crystals. Jeffrey J. Lovelace, Jason C. Porta, Gloria E.O. Borgstahl.

10:55-11:20 13.01.06
Predicting Possible Modulated Phases in the Layered Perovskite-like A_2BX_4 Structures of Propylammonium Tetrachlorometallates. Ian Swainson.

11:20-11:45 13.01.07
Disordered and Modulated Vanadium Oxide Structures. Peter Zavalij.

11:45-12:10 13.01.08
Study of Structure-property Relationship in Novel Inorganic Compounds with Disorder and/or Long Range Order. Olivier Gourdon, Delphine Gout, Gordon J. Miller, Thomas Proffen, Eric Bauer, Joe D. Thompson.

09.02 Macromolecular Dynamics
Joseph Curtis, 301B
Alec Sandy, Presiding

01:30-02:00 09.02.01
The Impact of Collective Molecular Dynamics on Physiological and Biological Functionalities of Artificial and Biological Membranes. Maikel Rheinstadter.

02:00-02:30 09.02.02
XPCS Studies of Nanoparticle Motion within Glassy Polymer Melts. Robert Leheny, Hongyu Guo, Gilles Bourret, R. Bruce Lennox, Mark Sutton, James Harden.

02:30-03:00 09.02.03
Dynamics of Threadlike Micelles Studied by Neutron Spin Echo. Dobrin Bossev, Wei-Ren Chen, Paul Butler, Lee Magid.

03:00-03:30 Coffee Break.

03:30-04:00 09.02.04
Protein Dynamics in the Crystalline State. Jeremy Smith.

04:00-04:30 09.02.05
Dynamical Coupling Between Hydration Water and Proteins: A Comparison of Membrane and Soluble Proteins. Kathleen Wood, Douglas Tobias, Giuseppe Zaccai, Martin Weik.

04:30-05:00 09.02.06
Comparison of Relaxation Dynamics in Saturated and Unsaturated Oriented Lipid Bilayers. Hirsh Nanda, Victoria Garcia-Sakai, Susan Krueger, Joseph E. Curtis.

13.02 Solid State Transformations and Reactions

Gracelia Diaz de Delgado, 301C
Marilyn Olmstead, Presiding

01:30-02:00 13.02.01
Concomitant Polymorphism and Twinning of Dichloro-bis(η^5 -tert-butylcyclopentadienyl)titanium(IV). Iliia Guzei, Hakon Hope, Amitabha Mitra.

02:00-02:30 13.02.02
The Syntax, Chemistry and Crystallography of Solid-state Reactions in Molecular Crystals: Visiting the Past to Understand the Present. Bruce M. Foxman.

02:30-03:00 13.02.03
Novel Supramolecular Approaches to Design Photoreactive Multi-component Assemblies: From Single to Concomitant Topochemical [2+2] Photoreactions. Alexander Briceno Villarreal.

03:00-03:30 Coffee Break.

03:30-04:00 13.02.04
Characterisation of Solid-state Structural Phase Transitions. Ross Angel, Eleda Johnson, Jing Zhao, Fabrizio Nestola.

04:00-04:30 13.02.05
Isotopic H/D Structural Phase Transition in Ammonium Copper Tutton Salt. Arthur Schultz, Paula Piccoli, Michael Hitchman, Charles Simmons.

04:30-05:00 13.02.06
Competitive Isomerization and Dimerization Reactions: A New Look at Stereochemical Requirements for [2+2] Addition. Shao-Liang Zheng, Oanh Pham, Cris Vande Velde, Milan Gembicky, Philip Coppens.

13.03 Structural Biology in Neurological Disorders

Ruslan Sanishvili, 301DE
Gergely Toth, Presiding

01:20-01:30 Introduction: Inaugural Session on Neurological Disorders. Ruslan Sanishvili.

01:30-02:00 13.03.01
Structural Neurology: A New Approach to the Understanding, Treatment and Prevention of Neurologic Disorders. Gregory A. Petsko, Dagmar Ringe.

02:00-02:30 13.03.02
Crystal Structure of JNK3 in the DFG Loop Out Conformation. Gergely Toth, Scott Lovell, Hidong Kim, Jing Wu, Kyle Powell, Hing Sham, Irene Griswold-Prenner.

02:30-03:00 13.03.03
From Folding on Ribosomes to Misfolding of Alpha-synuclein in Parkinson's Disease: Insights from NMR Spectroscopy. John Christodoulou.

03:00-03:30 Coffee Break.

03:30-04:00 13.03.04
Structural Insights Into Neuronal Transporters. Paul Shaffer, Eric Gouax.

04:00-04:30 13.03.05
Structures of Synaptic Proteins Neuroligin-1 and the Neuroligin-1/Neurexin-1 β Complex Reveal Specific Protein-protein and Protein-Ca²⁺ Interactions. Demet Arac, Antony A. Boucard, Engin Ozkan, Pavel Strop, Evan Newell, Thomas C. Sudhof, Axel T. Brunger.

04:30-05:00 13.03.06
Clinical and Pre-clinical Evaluation of Structure Based Phenylketonuria Therapeutics. Raymond Stevens.

MONDAY, JUNE 2

Rigaku Fun Run 07:15am World's Fair Park
Registration Desk 07:30am-05:30pm Henley Concourse
Speaker Ready Room 07:30am-05:30pm 301A
Council Meeting Room 07:30am-05:30pm Rontunda
Exhibit Show 10:00am-07:30pm Exhibit Hall B
BioMac SIG Meeting 12:00pm Ballroom C

Industrial SIG Meeting 05:00pm 301B
Small Molecule SIG Meeting 05:00pm Ballroom C
Neutron/Powder/Mats SIG 12:00pm 301C
Poster Session II 05:30pm-07:30pm Exhibit Hall B
Young Scientist Mixer 07:30-10:30pm Sunsphere
(ticket required)
Bruker AXS Party (by invitation only) 07:30-10:30pm

TR.01 Complementary Methods for Structure/Function Studies of Biomolecules

Susan Krueger, *301DE*

Carrie Wilmot, Presiding

Part I - Redox Chemistry and Associated Single Crystal Spectroscopies

08:30-09:10 TR.01.01
In Crystallo UV-visible Spectroscopy.
Dominique Bourgeois.

09:10-09:35 TR.01.02
Photoreduction of Metalloprotein Active Sites by Synchrotron Radiation. Britt Hedman, Mary C. Corbett, Matthew J. Latimer, Thomas L. Poulos, Irina F. Sevrioukova, Keith O. Hodgson.

09:35-10:00 TR.01.03
XANES Measurements of the Rate of Radiation Damage to Selenomethionine Side Chains. James Holton.

10:00-10:30 Coffee Break.

Part II - Neutron Methods

10:30-11:00 TR.01.04
Dynamics of Soluble and Membrane Proteins and their Surroundings. Douglas Tobias.

11:00-11:30 TR.01.05
Neutron Protein Crystallography.
Leighton Coates.

11:30-12:00 TR.01.06
Neutron Diffraction Studies of Membranes and Membrane Proteins as Multilayers. David Worcester, Ella Mihailescu, Stephen White.

12:00-01:30 Lunch Break.

Session continues after lunch at 01:30

01.02 Engage Your Brain

Raj Rajashankar, *Ballroom C*

Zbigniew Dauter, Presiding

08:30-09:00 01.02.01
Data Collection - Not Enough to Press the Button. Zbigniew Dauter.

09:00-09:30 01.02.02
Likelihood, Parameter Estimation, and Decision Making in Macromolecular Crystallography. Charles Carter.

09:30-10:00 01.02.03
It All Happens at Once - Magnitude Estimation of Uncertainty Components. Dominika Borek, Marcin Cymborowski, Wladek Minor, Zbyszek Otwinowski.

10:00-10:30 Coffee Break.

10:30-11:00 01.02.04
Phasing in Spite of Complications, and Sometimes Thanks to the Complications. Gerard Bricogne.

11:00-11:30 01.02.05
Juggling With Space Groups: Structure of a Fragment of the *Streptococcus mutans* Adhesin Antigen I/II. Champion Deiganayagam.

11:30-12:00 01.02.06
Macromolecular Crystal Structures Involving Non-Merohedral Twinning and/or Non-Crystallographic Translation. Kanagalaghatta Rajashankar.

04.01 Challenges in Industrial Crystallography

Jeff Bell, *301B*

Tim Rydel, Presiding

08:30-08:50 04.01.01
Crystal Structure of Synthetic Hydrotungstite, $WO_2(OH)_2(H_2O)$. James Kaduk, Judith Sentman.

08:50-09:10 04.01.02
Electron Crystallography in Petroleum Industrial Research. Douglas Dorset.

09:10-09:30 04.01.03
Charge Flipping Approach to Inorganic Structures from Powder Data. Scott Mixture.

09:30-09:50 04.01.04
2D-XRPD, a Powerful Tool for the Understanding of Various Defects in Sorel Cements. Robert Dinnebier, Kuniyoshi Sugimoto, Thomas Schlecht.

09:50-10:10 04.01.05
Chemical Crystallography as a Routine Analytical Tool for Preparative Chemists. Charles Campana, Bruce Becker, Stephen Leo, Greg Wachter, J. Kaercher, M. Ruf.

10:10-10:30 Coffee Break.

10:30-10:50 04.01.06
Trials and Tribulations in Pursuit of

Structure-Based Drug Design Targeted at MAPKAP Kinase-2. Ravi Kurumbail, N. Caspers, H.-S. Shieh, W. Stallings, G. Poda, J. Pawlitz, R. Broadus, M. Meyers, D. Anderson, R. Mourey, T. Stults, S. Bolten, R. Weinberg.

10:50-11:10 04.01.07
Overcoming Protein Expression, Purification and Crystallization Obstacles in Support of Structure-Based Drug Design in Industry. Melissa Harris, W. Brown, S. Foltin, J. Knafels, L. McDowell, J. Ohren, D. Omecinsky, Y. Xhu, R. Sarver, B. Finzel.

11:10-11:30 04.01.08
Crystallography as a Screening Tool: Challenges of Fragment Based Drug Discovery. John Spurlino, Frank Lewandowski, Cindy Milligan, Carsten Schubert, Marta Abad, Richard Alexander.

11:30-12:00 Round Table Discussion

13.04 Diffraction Studies of Correlated Electron Systems

Andrey Zheludev, Presiding *301C*

08:30-09:15 13.04.01
Magnetically Induced Ferroelectricity in Frustrated Quantum Magnets. Michel Kenzelmann.

09:15-10:00 13.04.02
Interplay Between the Short-Range Polar Order and Low-Frequency Lattice Dynamics in Relaxor Ferroelectrics. P.M. Gehring, C. Stock, G. Xu, W. Chen, Z.-G. Ye, H. Cao, J.-F. Li, D. Viehland, H. Luo.

10:00-10:30 Coffee Break.

10:30-11:00 13.04.03
Spin and Charge/orbital Ordering in Nearly Half-doped Manganites. Jaime Fernandez-Baca.

11:00-11:30 13.04.04
Short-range Charge and Spin Superlattices in Layered Perovskite Oxides. Igor Zaliznyak, Andrei Savici, Genda Gu, Hideki Yoshizawa, Naoki Sakiyama, Ying Chen, Hye Jung Kang.

11:30-12:00 13.04.05
Three Dimensional Magnetic Correlations in $LuFe_2O_4$. A.D. Christianson, M.D. Lumsden, M. Angst, Z. Yamani, W. Tian, R. Jin, S.E. Nagler, B.C. Sales, D. Mandrus.

TR.01 Complementary Methods for Structure/Function Studies of Biomolecules

Susan Krueger, *30IDE*
Carrie Wilmot, Presiding

Part III - Small Angle Scattering

01:30-02:10 TR.01.07
Combining High-Resolution Structures with Small-Angle Scattering and Neutron Contrast Variation Data for Studying of Protein Complexes in Solution. Jill Trehwella.

02:10-02:35 TR.01.08
Real-time Small-Angle X-ray Scattering Study of Assembly and Disassembly Cycles of Cyanobacterial Circadian Clock Proteins. Shuji Akiyama.

02:35-03:00 TR.01.09
Use of SAXS to Interrogate a Known Crystal Structure as a Basis for Modeling the HIV Defense Factor APOBEC3G. Joseph E. Wedekind, Jason D. Salter, Ryan P. Bennett, Jolanta Krucinska, Richard E. Gillilan, Harold C. Smith.

03:00-03:30 Coffee Break.

Part IV - Dynamics and Function (NMR/crystallography)

03:30-04:00 TR.01.10
Trapping an Invisible DNA Repair Intermediate for NMR and Crystallography. James Stivers.

04:00-04:30 TR.01.11
Merging Crystallography and Spectroscopy to Define Docking at the Proteasome via Rpn13. Kylie Walters.

04:30-05:00 TR.01.12
Structural Aspects of HIV-1 Entry Using NMR, X-ray Crystallography and Docking Techniques. Carole Bewley, Son Lam, Chih-Chin Huang, Priyamvada Acharya, Syed Hussan, Peter Kwong.

13.05 Modern Teaching Tools for 21st Century Science

Thomas Proffen, *Ballroom C*
Bernhard Rupp, Presiding

01:30-02:00 13.05.01
Educating Virtual APS Users: On-line Educational Materials for Powder Diffraction Crystallography. Brian Toby.

02:00-02:30 13.05.02
Crystallography and Scientific Inquiry. Bernhard Rupp.

02:30-03:00 13.05.03
An Interactive Tutorial to Teach Diffraction Physics Related to Crystal Structure Determination. Reinhard Neder.

03:00-03:30 Coffee Break.

03:30-04:00 13.05.04
Exploiting Advances in Cyberinfrastructure to Provide Practical Experience in Crystallography. K.A. Kantardjieff.

04:00-04:30 13.05.05
The Interactive Lectures for the School & College Instructors. Boris Kodess, Pavel Kodess, Felix Sidoreko, Petr Kodes, Polina Kodess.

13.06 Molecular Magnets

Jamie Manson, Presiding *301C*

01:30-02:05 13.06.01
Molecule-based Magnets: New Chemistry and New Materials for this Millennium. Joel Miller.

02:05-02:40 13.06.02
The Role of Halide-Halide Exchange Coupling in Low Dimensional Copper Halide Quantum Magnetic Systems. Roger Willett.

02:40-03:00 13.06.03
[4x4] Grids by Designed Self-Assembly: Mn^{II}_{16} , Cu^{II}_{16} , Co^{II}_{16} and Ni^{II}_{16} Magnetostructural Investigations. Louise Dawe, Laurence Thompson.

03:00-03:30 Coffee Break.

03:30-04:05 13.06.04
Hydrogen-Bonding and Exchange in Benzimidazole-Functionalized Organic Radical Solids. Paul Lahti.

04:05-04:35 13.06.05
Hydrogen Bond Mediated Magnetic Superexchange: Deuterium Isotope Effect in $CuF_2(H_2O)_2$ (pyrazine). John Schlueter, Kylee Funk, Jamie Manson, Sonal Brown, Janice Musfeldt.

04:35-05:00 13.06.06
Hydrogen Bonding and Multiphonon Structure in Copper Pyrazine Coordination Polymers. J.L. Musfeldt, S. Brown, M.M. Conner, A.C. McConnell, H.I. Southerland, J.L. Manson, J.A. Schlueter, M.D. Phillips, M.M. Turnbull, C.P. Landee.

13.07 Professional Directions

Bobby Huether, Presiding *301B*
01:30-5:00

The "Professional Directions" session, organized by the Young Scientist and Service Special Interest Groups, will provide an informal opportunity for young scientists to interact with established scientists and discuss career-related issues. The panel will be convened to discuss current opportunities for young scientists in both traditional and non-traditional scientific professions, and is aimed at graduate students, post-doctoral fellows, and young professors. The goal of the session is to provide young scientists both with a current snapshot of a "day in the life" of a professional scientist, and also an opportunity to provide practical information for graduate students and post-doctoral candidates undecided as to their career path. The panel members are Gregory Petsko (Brandeis University), David Rose (University of Toronto), Jane Richardson (Duke University), and Jeanette Krause (University of Cincinnati). All are welcome to attend and contribute to the conversation!

TUESDAY, JUNE 3

Registration Desk 07:30am-05:30pm..... Henley Concourse
Speaker Ready Room 07:30am-05:30pm..... 301A
Council Meeting Room..... 07:30am-05:30pm..... Rontunda
Exhibit Show 10:00am-07:30pm..... Exhibit Hall B
Synchrotron SIG Meeting 12:00pm 301DE
Canadian Div. Meeting 12:00pm 301B

SAS SIG Mtg 12:00pm 301C
Fiber SIG Meeting 04:40pm 301B
Service SIG Meeting 05:00pm 301DE
Poster Session III 05:30pm-07:30pm..... Exhibit Hall B
Rayonix Party 07:30pm-12:00am
Mentor/Mentee Dinner 07:30-10:30pm Calhoun's
(ticket required) 400 Neyland Dr.

01.03 Difficult Structures

Tom Smith, *Ballroom C*
Dinesh Yernool, Presiding

08:30-08:55 01.03.01
X-ray Structure of the Zinc Transporter YiiP.
Min Lu, Dax Fu.

08:55-09:20 01.03.02
Crystal Structure of the Maltose Transporter.
Jue Chen, Michael Oldham, Dheeraj Khare,
Florante Quiocho, Amy Davidson.

09:20-09:45 01.03.03
A Virus Structure Determined at 3.8Å with
Less Than one Third of the Data Reveals
Evolution in Action. Jeffrey A. Speir, D. J.
Taylor, F.M. Pringle, L. Andrew Ball, J.E.
Johnson.

09:45-10:10 01.03.04
Hybrid LRR Technique and Crystal Structures
of the Toll-like Receptor Complexes.
Jie-Oh Lee.

10:10-10:40 Coffee Break.

10:40-11:05 01.03.05
A Plant Photosystem I Design in the Light
of Evolution. Alexey Amunts, Omri Drory,
Nathan Nelson.

11:05-11:30 01.03.06
Structure Determination of S_{MK} Riboswitch
via Microcrystallography. Changrui Lu,
Kanagalaghatta Rajashankar, Fang Ding,
Tina Henkin, Ailong Ke.

11:30-11:55 01.03.07
Structure of a β 1 Adrenergic Receptor:
Progress in Obtaining Recombinant G
Protein Coupled Receptor Structures.
Gebhard Schertler.

13.08 Catalysis Studies using SAXS and High Energy Scattering with PDF

Peter Chupas, *301B*
Randall Winans, Presiding

08:30-09:00 13.08.01
Resonant X-ray PDF Studies of Catalytic
Gold Nano-Particles. Takeshi Egami, Wojtek
Dmowski, Sheng Dai, Steve Overbury.

09:00-09:30 13.08.02
In situ Grazing Incidence Small Angle X-ray
Scattering: An Advanced Characterization
Technique for Catalyst Surfaces. Christine
Revenant, F. Leroy, G. Renaud, R. Lazzari,
A. Letoublon, T. Madey.

09:30-10:00 13.08.03
In-situ Combined GISAXS and TPR
Studies of Size Selected Nanocatalysts: A
New Approach to Investigate Size Effects in
Catalysis. Sungsik Lee, Yu Lei, Byeongdu
Lee, Randall Winans, Kristian Sell, Ingo
Barke, A. Kleibert, Viola von Oyenhhausen,
Karl-Heinz Meiwes-Broer, S. Vajda.

10:00-10:30 Coffee Break.

10:30-11:00 13.08.04
Combining WAXS/(SAXS) with Spectro-
scopic Measurements to Follow Catalysts in
Action. Andrew Beale, Bert Weckhuysen.

11:00-11:30 13.08.05
Watching Nanoparticles Grow: The Mechan-
ism and Kinetics for the Formation of TiO₂-
Supported Platinum Nanoparticles. Karena
Chapman, Peter Chupas, Guy Jennings,
Peter Lee, Clare Grey.

11:30-12:00 13.08.06
Solution Phase X-ray Scattering: Structural
Characterization of Supramolecular Por-
phyrin Assemblies. Karen Mulfort, Suk
Joong Lee, David Tiede, Joseph Hupp.

13.09 Emerging Opportunities for X-ray and Neutron Scattering: New Sources & New Techniques

Ken Herwig, *301DE*
Bob Sweet, Presiding

08:30-09:00 13.09.01
Synchrotron Science at SLAC/Stanford -
the LCLS and Other Recent Developments.
Keith Hodgson.

09:00-09:30 13.09.02
Coherence and Ultra-short Pulses for
Structure Determination: New Storage Ring
and FEL Facilities at DESY in Hamburg;
Petra-III, FLASH, and XFEL. Jochen
Schneider.

09:30-10:00 13.09.03
No Abstract. Steve Dierker

10:00-10:30 Coffee Break.

10:30-11:00 13.09.04
Serial Crystallography for the Cornell ERL.
John Spence, Bruce Doak, Uwe Weierstall,
Kevin Schmidt, Petra Fromme, Daniel De
Ponte, Richard Kirian, Mark Hunter, Henry
Chapman, David Shapiro.

11:00-11:30 13.09.05
New X-ray Scattering Opportunities With
an Upgraded Advanced Photon Source.
Dennis M. Mills.

11:30-12:00 13.09.06
Bigger, Better, Faster, More: The ESRF
Upgrade Programme. Edward Mitchell, on
Behalf of the ESRF.

Session continues after lunch @ 01:30pm

13.10 Supramolecular Chemistry: Organic Crystals from Assembly to Function

Jennifer Swift, Presiding *301C*

08:30-08:40 Introduction.

08:40-09:20 13.10.01
More about Eligio Perucca, Primo Levi,
Induced Optical Activity, and Enantio-
selective Adsorption to Crystals. Bart Kahr,
Yonghong Bing, John Freudenthal, Werner
Kaminsky, Davide Viterbo.

09:20-09:40 13.10.02
Correlation of Biomineral Crystal Growth
Modification with Impurity Adsorption
Kinetics. Ryan Sours, Randall Mazzarino,
Tissa Thomas.

09:40-10:00 13.10.03
Surface and Microwave Methods for the
Selection of Pharmaceutical Polymorphs.
Venkat R. Thalladi.

10:00-10:30 Coffee Break.

10:30-11:10 13.10.04
What do Polymorphs Teach us About
Crystal Nucleation and Growth? Lian Yu,
Jing Tao, Sun Ye, Hanmi Xi, Shuang Chen,
Jun Huang, Mark Ediger.

11:10-11:50 13.10.05
Cross-nucleation and Polymorph Selection:
Unravelling the Competition Between
Kinetics and Thermodynamics. Jerome
Delhommelle, Caroline Desgranges.

11:50-12:10 13.10.06
An *in situ* Atomic Force Microscopy Study
of Monosodium Urate Crystal Growth.
Clare M. Yannette, Jennifer A. Swift.

Session continues after lunch @ 01:40pm

01.04 Structural Enzymology

Allen Orville, *Ballroom C*
Carrie Wilmot, Presiding

01:30-01:55 01.04.01
Insights into Blue-light Photoreceptors - How to BLUF. Ilme Schlichting.

01:55-02:15 01.04.02
CoA As Catalyst: A Detailed Study of Hydride Transfer in HMG-CoA Reductase. C. Nicklaus Steussy, C.J. Duncan, T. Schmidt, L.V. Wrensford, J.W. Brugner, V. W. Rodwell, C.V. Stauffacher.

02:15-02:40 01.04.03
Structures of Cytochrome *c* Oxidase Reveal a Conformational Change upon Reduction and a Steroid Binding Site, Both Impacting the K Proton Path. Shelagh Ferguson-Miller, L. Qin, D. A. Mills, C. Hiser, R.M. Garavito.

02:40-03:00 01.04.04
Structure Based Enzymology of the Formation of Several Intermediates from the Thiamin Biosynthetic Enzyme Thi4 in *Saccharomyces cerevisiae*. Christopher Jurgenson, Abhishek Chatterjee, Amrita Hazra, Frank Schroeder, Ying Han, Tadhg Begley, Steven Ealick.

03:00-03:30 Coffee Break.

03:30-03:55 01.04.05
An Interlocked Dimer of the Protelomerase TelK Distorts DNA Structure for the Formation of Hairpin Telomeres. Tom Ellenberger.

03:55-04:15 01.04.06
Insight into the Mechanism of the Cofactorless Urate Oxidase: X-ray Structures with Molecular Oxygen and with the Dehydrourate Intermediate. Nathalie Colloc'h, Laure Gabison, Guillaume Marassio, Jacques Abraini, Mohamed Chiadmi, Thierry Prange.

04:15-04:40 01.04.07
Ruffling of Metalloporphyrins Bound to the Heme Degrading Enzymes IsdG and IsdI. Michael Murphy, Woo Cheol Lee, Georgi Ukpabi, Michelle Reniere, Eric Skaar.

04:40-05:00 01.04.08
Observation of a Flavin-C4a-Oxygen Intermediate by Crystallographic, Spectroscopic, and Computational Methods. Allen Orville, Rajeev Prabhakar, George Lountos, Steffan Finnegan, Giovanni Gadda.

02.01 Fiber Diffraction & Friends (compl. Neut/X-ray + EM, SAS, etc)

Joseph Orgel, *301B*
Gerald Stubbs, Presiding

01:30-02:00 02.01.01

Fiber Diffraction and Cryo-electron Microscopy Applied to Filamentous Viruses. Gerald Stubbs, Amy Kendall, Wen Bian, Michele McDonald, Sarah Baumgarten, Timothy Bowles, Jian Shi, Phoebe Stewart.

02:00-02:20 02.01.02
Polyproline Changes Threshold Polyglutamine Length in Fibril Formation. Greg Darnell, Joseph Orgel, Stephen Meredith.

02:20-03:00 02.01.03
Studies of Amyloid and Amyloid-related Structures in Natural Fibres and Virus-derived Peptide Sequences. V. Trevor Forsyth, S. Tiggelaar, E. Mossou, M. Kasotakis, P. Callow, K. Gardner, R. Denny, E. Mitchell, A. Mitraki.

03:00-03:30 Coffee Break.

03:30-03:50 02.01.04
Iota-carrageenan: A Paradigm of Cation Dependent Polymorphism, Pseudopolymorphism and Molecular Heterogeneity. Rengaswami Chandrasekaran, Srinivas Janaswamy.

03:50-04:20 02.01.05
Molecular Structure, Ligand Binding and Collagenolysis of the Native Type I Collagen Fibril. Joseph Orgel, James San Antonio, Shawn Sweeney, Rong Wang, Shiamalee Perumal, Olga Antipova.

04:20-04:40 02.01.06
Molecular Structure of the Native Type II Collagen Fibril. Olga Antipova, Kalpana Ramakrishnan, Dengli Qiu, Rong Wang, Joseph Orgel.

04:40 Fiber Diffraction SIG Meeting.

13.09 Emerging Opportunities for X-ray and Neutron Scattering: New Sources & New Techniques

Ken Herwig, *301DE*
Bob Sweet, Presiding

01:30-02:00 13.09.07
Facilities for X-ray Scattering, Diffraction, and Crystallography at the Canadian Light Source. Michel Fodje.

02:00-02:30 13.09.08
DIAMOND: Diffraction and Many Other New Directions for UK Science. Elizabeth Duke.

02:30-03:00 13.09.09
Neutron Scattering Opportunities at ORNL's New and Upgraded Neutron Facilities: The Spallation Neutron Source and High Flux Isotope Reactor. Kenneth Herwig.

03:00-03:30 Coffee Break.

03:30-04:00 13.09.10
Two Novel Reflectometers for the Expanded NCNR Cold Neutron Guide Hall: CANDoR and MAGIK. Brian B. Maranville, Charles Majkrzak, Norman Berk.

04:00-04:30 13.09.11
Recent Developments at the ISIS Facility. Richard M. Ibberson.

04:30-04:45 13.09.12
Time Resolved Atomic-Resolution Laue Studies at the AR Ring at KEK. Mateusz Pitak, Milan Gembicky, Shao-Liang Zheng, Philip Coppens, Marc Messerschmidt, Shin-Ichi Adachi, Shin-Ya Koshihara.

04:45-05:00 13.09.13
Macromolecular Powder Diffraction: Structure Solution via Molecular Replacement. Jennifer Doebbler, Robert Von Dreele.

13.10 Supramolecular Chemistry: Organic Crystals from Assembly to Function

Jennifer Swift, Presiding *301C*

1:40-02:20 13.10.07
Reaction Crystallization Mechanisms for Screening and Synthesis of Cocrystals. Nair Rodriguez-Hornedo, Sarah Nehm, Adivaraha Jayasankar, D. Good, L. Sreenivas Reddy.

02:20-02:40 13.10.08
Polymorphism and Isomer Cocrystals of Dimers of Phenylpropioyl Chloride. Raymond E. Davis, Vincent M. Lynch.

02:40-03:00 13.10.09
An Unexpected Co-Crystal with a Variable Degree of Order: 1:1 rac-1,2-Cyclohexanediol/Triphenylphosphine Oxide. Carolyn Brock, Maxime A. Siegler, Yigang Fu, Greg H. Simpson, Daniel P. King, Sean Parkin.

03:00-03:30 Coffee Break.

03:30-04:10 13.10.10
A Thermodynamic Understanding of the Stability of Co-Crystals. Matthew Peterson, Mark Oliveira, Roger Davey.

04:10-04:30 13.10.11
Managing Supramolecular Assemblies using Molecular Shape. Kraig Wheeler.

04:30-05:10 13.10.12
Formation and Characterization of Polymer-Reinforced Porous Single Crystals. Lara Estroff, Hanying Li, Miki Kunitake.

Session continues Wednesday at 01:40pm

WEDNESDAY, JUNE 4

Registration Desk 07:30am-05:30pm Henley Concourse
 Speaker Ready Room 07:30am-05:30pm 301A
 Council Meeting Room ... 07:30am-05:30pm Rontunda

Young Scientist SIG Meeting 12:00pm 301DE
 ACA All Member Business Meeting 05:00pm Ballroom C
Awards Banquet Convention Center
 Cash Bar 6:30pm Dinner 07:30pm (ticket required)

AW.01 Etter Early Career Award Symposium**Anna Gardberg, Presiding 301DE**

08:30-08:35 Presentation of Award to Radu Custelcean. Marvin Hackert, ACA President.

08:35-09:15 AW.01.01
 Manipulating Hydrogen Bonds in Crystalline Solids: From Etter's Rules to Anion Recognition. Radu Custelcean.

09:15-09:30 AW.01.02
 Crystal Growth of Bis-Diphenyl Ureas on Silica Templates. Christina A. Capacci, Jennifer A. Swift.

09:30-09:45 AW.01.03
 Synthesis of Materials in the AA'W₃O₁₂ Family using a Non-Hydrolytic Sol-Gel Process. Tamam Baiz, Cora Lind.

09:45-10:00 AW.01.04
 Adventures in Fullerene Crystallography: A Basketful of Egg-shaped Fullerenes and a Glimpse of What May Come. Christine M. Beavers, Marilyn M. Olmstead, Christopher J. Chancellor, Alan L. Balch.

10:00-10:30 Coffee Break.

10:30-10:35 Presentation of Etter Student Lecturer Award to Aruna Shankaranarayanan, Univ. of Michigan.

10:35-11:00 AW.01.05
 Structural Insights into the Activation of RhoA by G_i Coupled Receptors. Aruna Shankaranarayanan, Susanne Lutz, Cassandra Coco, Marc Ridilla, Mark R. Nance, Christiane Vettel, Doris Baltus, Richard R. Neubig, Thomas Wieland, John Tesmer.

11:00-11:20 AW.01.06
 Cholix Toxin, a Novel ADP-ribosylating Factor from *Vibrio cholerae*. Rene Jorgensen, Alexandra E. Purdy, Robert J. Fieldhouse, Matthew S. Kimber, Douglas H. Bartlett, A. Rod Merrill.

11:20-11:40 AW.01.07
 A New Detergent System for Membrane Protein Crystallization: 1.4 Å Crystal Structure of the Membrane Protein PagP in SDS/MPD. Jose Antonio Cuesta-Seijo, Gilbert Prive.

11:40-12:00 AW.01.08
 ER α -Glucosidase I: Expression, Purification, and Preliminary Crystallography. Megan Barker, David Rose.

01.05 Computational Crystallography - Nuts and Bolts

Acknowledgement is made to Area Detector Systems, Corp. for partial support of this session

**Ed Collins, Ballroom C
 Peter Horanyi, Presiding**

08:30-09:00 01.05.01
 Macromolecular Crystal Diffraction Data Collection: Opinions about Best Practices. James Pflugrath.

09:00-09:30 01.05.02
 Introduction to Experimental Phasing of Macromolecules. George M. Sheldrick.

09:30-10:00 01.05.03
 Tools for Easy and Difficult Problems: Automation of Structure Determination. Thomas Terwilliger.

10:00-10:30 Coffee Break.

10:30-11:00 01.05.04
 Paul Emsley.

11:00-11:30 01.05.05
 Using Local Validation to Improve Your Structure and Streamline its Completion. David Richardson, Jane Richardson.

11:30-11:45 01.05.06
 Some Effects of Experimental Error on Substructure Determination. Hongliang Xu, Charles M. Weeks.

11:45-12:00 01.05.07
 Incorporating Stereochemical Restraints in a Resolution Dependent Manner. Dale Tronrud.

03.01 General Interest I**Allen Oliver, Presiding 301B**

08:30-09:00 03.01.06
 Synthesis, Structures, Morphologies and Optical Properties of Some New Chiral Thiocarbamates and Thioureas. Werner Kaminsky, D. Responte, D. Daranciang, J. Gallegos.

09:00-09:30 03.01.01
 Two Men and a Genome: A Poor Man's Approach to Structural Genomics. Joseph D. Ng, Ronny C. Hughes, Miranda L. Byrne, Damien Marsic.

09:30-10:00 03.01.02
 Selenium Derivatization of Nucleic Acids for Phasing and Crystallization in Crystallography. Zhen Huang, Jiansheng Jiang, Jia Sheng, Nicolas Carrasco.

10:00-10:30 Coffee Break.

10:30-11:00 03.01.03
 An Example of Successful Sulfur SAS Phasing using Medium-Resolution Data: Crystal Structure of *Archaeoglobus fulgidus* ORF 1382. Jin-Yi Zhu, Z-Q. Fu, Lirong Chen, Hao Xu, John

Chrzas, John Rose, Bi-Cheng Wang.

11:00-11:30 03.01.04
 New Optics for Macromolecular Crystallography. Kris Tesh, A. Criswell, L. Jiang, B. Simpson, B. Verman, C. Yang, J. Ferrara.

11:30-12:00 03.01.05
 Automating Crystallography (somewhat) from Start to Finish. Joel Bard, Mark Johnson, Kristine Svenson, Erik Vogan, Kevin Parris, Lydia Mosyak, Will Somers.

13.11 Biological Applications of SAXS and SANS**William Heller, 301C
 Greg Hura, Presiding**

08:00-08:30 13.11.01
 Small Angle Scattering Studies of Cationic Driven Folding of RNA. Robert Briber, S. Moghaddam, J.-H. Roh, G. Caliskan, S. Chauhan, R. Behrouzi, D. Thirumalai. S. Woodson.

08:30-09:00 13.11.02
 Combining Small Angle Scattering and NMR Restraints for Structural Refinement of Macromolecular Complexes in Solution. Frank Gabel.

09:00-09:30 13.11.03
 Analyzing Flexible Proteins Using Small Angle X-ray Scattering. Efstratios Mylonas, Pau Bernado, Maxim Petoukhov, Dmitri I. Svergun.

09:30-10:00 13.11.04
 Biological Small Angle Scattering/Diffraction Facility Beamline 4-2 at SSRL. Thomas M. Weiss, Marc Niebuhr, Ping Liu, Hiro Tsuruta.

10:00-10:30 Coffee Break.

10:30-11:00 13.11.05
 Resolution of the Unfolded State. Gregory Beaucage.

11:00-11:30 13.11.06
 SAXS Validation of Molecular Dynamics and Docking Based Conformational Sampling. Michal Hammel, Kenneth Frankel, Martin Pelikan, R. Rambo, G. Hura, John Tainer.

11:30-12:00 13.11.07
 Molecular Envelopes from SAXS and Single-Molecule Diffraction Experiments at an XFEL. Dilano Saldin, Valentin Shneerson, Russell Fung, Abbas Ourmazd.

12:00-12:30 13.11.08
 Crystallographic and Small Angle Scattering Studies of the Bacteriophage T4 Replication Complex. Jennifer Hinerman, Leif Hanson, Timothy Mueser.

**AW.02 Patterson Award
Advances in Macromolecular
Phasing & their Impact to
Structural Biology**

Gary Newton, *30IDE*
John Rose, Presiding

01:30-01:35 Presentation of Award
to Bi-Cheng Wang. Marvin Hackert,
ACA President

01:35-02:20 AW.02.01
Resolution of Phase Ambiguity in
Macromolecular Crystallography: 25
Years Later. Bi-Cheng Wang.

02:20-02:45 AW.02.02
Evolution of Phase Evaluation from
MAD and SAD Measurements. Wayne
A. Hendrickson.

02:45-03:10 AW.02.03
Wang Limit. Zbyszek Dauter.

03:10-03:30 Coffee Break.

03:30-03:55 AW.02.04
S and Cr, the Power Couple Next Door.
Emil F. Pai, Yan Liu, Aiping Dong.

03:55-04:20 AW.02.05
Neutron Direct Methods: Have Structure
Applications Involving Neutrons Come of
Age? David Langs, Herbert Hauptman.

04:20-04:45 AW.02.06
Direct Methods and Solvent Flattening.
Hai-fu Fan.

04:45-05:10 AW.02.07
Molecular Machines, Tropical Diseases
and the Power of llamas. Wim G. J. Hol.

05:10-05:35 AW.02.08
The First *denovo* Structure Determinations
using Wang's ISAS Technique. John
Rose.

**01.06 Systematic Molecular
Anatomy, Structural Phylogeny,
and Evolution**

Charlie Carter, *Ballroom C*
Bill Duax, Presiding

01:30-02:00 01.06.01
Building a Structural Phylogeny of the
SCOR Binding Pocket. Robert Huether,
Vladimir Pletnev, Timothy Umland, Charles
M. Weeks, Sanjay Connare, W. Duax.

02:00-02:30 01.06.02
Combining Protein Sequence and X-
Ray Structure to Trace 3 Billion Years of
Molecular Evolution. W. Duax, E. Huether,
V. Pletnev, S. Connare.

02:30-03:00 01.06.03
Statistical Evaluation of the Rodin-Ohno
Hypothesis: Sense/Antisense Coding of
Ancestral Class I and II Aminoacyl-tRNA
Synthetases. G. Gurkan Yardimci.

03:00-03:30 Coffee Break.

03:30-04:00 01.06.04
Crystal Structure of an Ancient Protein:
Evolution by Architectural Epistasis. Eric
Ortlund, Jamie Bridgham, Joseph Thornton,
Matthew Redinbo.

04:00-04:30 01.06.05
Enzymological Characterization of the
TrpRS Minimal Catalytic Domain. Yen
Pham, Charles Carter.

04:30-05:00 01.06.06
The Structural Basis of Ribozyme-Catalyzed
RNA Assembly. Michael P. Robertson,
William G. Scott.

**13.10 Supramolecular Chemis-
try: Organic Crystals from
Assembly to Function**

Jennifer Swift, Presiding *30IC*

01:40-02:20 13.10.13
Serendipity in Drug Development: Dis-
covery and Development of Stable
Crystalline Forms of Active Pharmaceutical
Ingredients. Narayan Variankaval.

02:20-02:40 13.10.14
Structure and Thermal Behavior of Metal
Citraconates. Graciela Díaz de Delgado,
Teresa González, Alexander Briceño.

02:40-03:00 13.10.15
Structural and Magnetic Properties of
[Cu(HF₂(pyrazine)₂)]SbF₆ and a Defect-
rich Analog [Cu₂F(HF)(HF₂(pyrazine)₄)](S
bF₆)₂. Jamie Manson, Heather Southerland,
Brendan Twamley, John Schlueter, Kylee
Funk.

03:00-03:30 Coffee Break.

03:30-04:10 13.10.16
Architectural Diversity and Elastic Networks
in Hydrogen-bonded Host Frameworks:
From Molecular Jaws to Cylinders to
Embedded Capsules. Michael Ward.

04:10-04:30 13.10.17
Metallosupramolecular Architectures Based
on Metal(II)-betadiketonates and Small
Polyfunctional Molecules as Building
Blocks. Nenad Judaš.

04:30-04:50 13.10.18
Crystallisation Methods for the Synthesis of
Coordination Polymer Complexes. Elinor
Spencer, Judith Howard.

04:50-05:10 13.10.19
Hydrolysis of PF₆⁻ as a Route to Uranium
Phosphates. Nicholas Deifel, K. Travis
Holman, Christopher L. Cahill.

**13.12 Powder Challenges:
Structures Under Nonambient
Conditions**

Chris Tulk, Presiding *30IB*

01:30-02:15 13.12.01
Electron Density at High Pressure From
Maximum Entropy. John Tse.

02:15-03:00 13.12.02
Structural Changes in Nano-crystalline
Mackinawite (n-FeS) at High-pressure.
Lars Ehm, Marc Michel, Sytle Antao, Peter
Chupas, Peter Lee, David Martin, Sarvjit
Shastri, John Parise.

03:00-03:30 Coffee Break.

03:30-03:50 13.12.03
Guest Atom Disorder in sII and sH Krypton
Clathrate Hydrates. Bryan Chakoumakos,
Ling Yang, D.D. Klug, C.A. Tulk, D. Martin,
Lars Ehm, J.B. Parise.

03:50-04:10 13.12.04
A New Hexagonal Phase for Pressure-
Quenched Xe Clathrate Hydrate. L. Yang,
C. A. Tulk, D.D. Klug, L. Ehm, D. Martin,
B.C. Chakoumakos, J.J. Molaison, J.B.
Parise.

04:10-04:40 13.12.05
High Energy X-ray Diffraction from
Aerodynamically Levitated Silicate Melts.
Chris Benmore, Martin Wilding, Richard
Weber, Qiang Mei.

**All Member
Business Meeting
Ballroom C
at 05:00pm**

01.07 How Structures are Used by Others**Eric Bennett,** *Ballroom C*
Roland Dunbrack, Presiding08:30-09:15 01.07.01
What Do Other People Want from Your Crystal Structure? Jane Richardson, David Richardson.09:15-10:00 01.07.02
Statistical Analysis of Protein Structures: Electron Density, Conformational Analysis, and Protein-protein Interfaces. Roland Dunbrack, Maxim Shapovalov, Qifang Xu, Daniel Ting, Michael Jordan.

10:00-10:30 Coffee Break.

10:30-11:00 01.07.03
Dramatic Changes of Protein Structure in Evolution. Nick Grishin.11:00-11:30 01.07.04
Sampling Slow Conformational Switches in Proteins. Donald Hamelberg, J. Andrew McCammon.11:30-12:00 01.07.05
Computational Prediction of Structures of Protein Complexes and Multi-domain Proteins. Jeffrey Gray.**10.01 Cool Structures****Allen Oliver, Presiding** *301C*08:30-08:50 10.01.01
Using X-ray and Neutron Diffraction to Study Complexes of Cyanuric Acid with Group I Metals: Neutron Crystallography from an X-ray Perspective. Gary Nichol, William Clegg, Matthias Gutmann, Duncan Tooke.08:50-09:10 10.01.02
Novel Cationic Copper Coordination Networks Constructed from 4, 4'-Bis-imidazolylbiphenyl Ligand. Liangming Hu, Elinor Spencer, Carla Slebodnick, Brian Hanson.09:10-09:30 10.01.03
Pressure Induced Coordination Changes in K-Co-Oxomolybdates. Jens Michael Engel, Hans Ahsbahs, Helmut Ehrenberg, Hartmut Fuess.09:30-09:50 10.01.04
Structural Variation within Homo- and Heterometallic Uranium(VI) Phosphonocarboxylates. Karah E. Knope, Christopher L. Cahill.

09:50-10:30 Coffee Break.

10:30-10:50 10.01.05
Structural Studies of Lanthanide Binolate Complexes Important as Catalysts in Asymmetric Synthesis. Patrick Carroll.10:50-11:10 10.01.06
Complex Packing Motifs Encountered in a Beta-cyclodextrin/adamantine Inclusion Compound. Gary Enright, Konstantin Udachin, John Ripmeester.11:10-11:30 10.01.07
New Hosts for Fullerenes. Marilyn Olmstead, Jimmy Franco, Justin Hammons.11:30-11:50 10.01.08
Crystal Packing in the Thiirane-based Gelatinase Inhibitor (S)-4-(4-(thiiran-2-yl-methylsulfonyl)phenoxy)phenyl Methanesulfonate, a System with Z'=6. Bruce C. Noll, Mijoon Lee, Dusan Heseck, Mayland Chang, Shahriar Mobashery.**13.13 Materials for Energy Applications****Craig Brown,** *301B*
Jason Hodges, Presiding08:30-09:10 13.13.01
The Prediction of Structure and Properties for Rechargeable Li Battery Electrode Materials. Gerbrand Ceder.09:10-09:35 13.13.02
Bulk Materials for Thermoelectric Power Generation. Michael McGuire.09:35-10:00 13.13.03
Structural Aspects of Coordination Polymers for Gas Storage. Craig Brown, Yun Liu, Dan Neumann.

10:00-10:30 Coffee Break.

10:30-10:55 13.13.04
Temperature and Pressure Dependent Structural Changes of MIL-53, A Potential H₂ Storage Material. Jae-Hyuk Her, Yun Liu, Craig Brown, Dan Neumann, Anne Dailly.10:55-11:20 13.13.05
Methane Storage in Nanoporous Metal-Organic Frameworks and Novel Phase Transition of Confined Methane. Hui Wu.11:20-11:40 13.13.06
Crystal Chemistry, Crystallography, and Thermoelectric Properties of Compounds in the Ca-Sr-Co-O System. W. Wong-Ng, G. Liu, E. Thomas, M. Otani, N. Lowhorn, J.A. Kaduk.11:40-12:00 13.13.07
Structure of a Fluorous Metal-Organic Framework with High Gas Storage Capacities. Xiaoping Wang, Chi Yang, Mohammad A. Omary.**13.14 Microcrystals****Richard Gillilan,** *301DE*
Ruslan Sanishvili, Presiding

08:15-08:30 Introduction: The State of Microcrystallography. Richard Gillilan.

08:30-09:00 13.14.01
in situ Study of Nanotemplate-Induced Growth of Protein Microcrystals by Submicron GISAXS. Claudio Nicolini, Sailish Tripathi, Eugenia Pechkova.09:00-09:30 13.14.02
High Resolution Electron Dffraction of 3D Protein and Pharmaceutical Nano-crystals. J.P. Abrahams, D. Georgieva, H.W. Zandbergen, S. Nicolopoulos, J. Portillio.09:30-10:00 13.14.03
Recording Data from Multiple Protein Microcrystals Using Laue Diffraction. Sterling Cornaby, David Schuller, Doletha M. E. Szebenyi, Detlef Smilgies, Quan Hao, Donald Bilderback.

10:00-10:30 Coffee Break.

10:30-11:00 13.14.04
ADedicated Tuneable Microfocus Beamline at Diamond Light Source: Prospects for Microcrystallography on Membrane Proteins. Gwyndaf Evans, Armin Wagner.11:00-11:30 13.14.05
Protein Crystallography with a Micrometre-sized Synchrotron-radiation Beam. Gebhard Schertler.11:30-12:00 13.14.06
Can Radiation Damage be Reduced with a 1-Micron Beam? Robert F. Fischetti, Ruslan Sanishvili, Derek Yoder, Stefan Vogt, Gerold Rosenbaum, V. Nagarajan, M. Becker, S. Xu, J.L. Smith

01.08 Practical Approaches to Improving the Formation and Diffraction-quality of Protein Crystals

George DeTitta, Ballroom C
Joe Luft, Presiding

01:30-02:00 01.08.01
Target Evaluation Coupled with Salvage Pathways to Increase Success Rates for Protein Production & Crystallization. Ian A. Wilson.

02:00-02:30 01.08.02
The Importance of Nucleation and Seeding in Protein Crystallization Case Studies using Microseed Matrix Seeding. Allan D'Arcy, Frederic Villard.

02:30-03:00 01.08.03
Order from Chaos - The Design and Interpretation of High-throughput Crystallization Screens to Guide Optimization. Edward Snell, Ray Nagel, Joseph Luft, Ann Wojtaszczyk, Meriem Said, Jennifer Wolfley, M. Elizabeth Snell, Melvin Parker, George DeTitta.

03:00-03:30 Coffee Break.

03:30-04:00 01.08.04
Screening for New Ligands; A Key to Higher Protein Crystallization Success Rate. Masoud Vedadi, Abdellah Allali-Hassani, Guillermo Senisterra, G. Wasney, P. Finerty, A. Edwards, C. Arrowsmith.

04:00-04:30 01.08.05
Solubility Screen to Improve Crystallization Trials and a Two Step Approach to Uncoupling Crystal Condition Searches. Timothy Mueser, Aude Izaac, Raj Gosavi, Constance Schall.

04:30-05:00 01.08.06
Macromolecular Crystal Annealing: Updating Techniques and Understanding Variables. Leif Hanson, Unmesh Chinte, Binal Shah, Raj Gosavi, Jennifer Hinerman, Constance Schall.

03.02 General Interest II

Peter Müller, 301B
Allen Oliver, Presiding

01:30-02:00 03.02.01
In Pursuit of the Trouble-Free Photon: Low Maintenance, High Brilliance X-ray Sources for the Home Lab. Matthew Benning, Anita Coetzee, Arjen Storm, Bram Schierbeek.

02:00-02:30 03.02.02
Translational and Rotational Calibration of Stationary Area Detectors. Joerg Kaercher, Michael Ruf.

02:30-03:00 03.02.03
Small X-ray Beams for Small Crystals: Pushing the Limits of Home-lab X-ray Sources. Jorg Wiesmann, Jorgen Graf, Carsten Michaelsen, Thomas Schulz, Dietmar Stalke.

03:00-03:30 Coffee Break.

03:30-04:00 03.02.04
Cluster Analysis in Crystallography. Chris Gilmore, Gordon Barr, Wei Dong, Andy Parkin, Chick Wilson.

04:00-04:30 03.02.05
Anomalous Dispersion for Dummies. Carla Slebodnick.

04:30-05:00 03.02.06
A Comparison of Bayesian and Flack Parameter Approaches for Organic Absolute Structure Determination. Ian D. Williams, Herman H-Y. Sung.

13.15 Diffuse Scattering Studies of Local Structure in the Solid State

Branton Campbell, 301DE
Thomas Proffen, Presiding

01:30-02:00 13.15.01
Interplay of Spin-orbital-charge and Lattice Degrees of Freedom in Cobaltites. Despina Louca.

02:00-02:30 13.15.02
Diffuse Scattering Studies of Local Structure in Crystals with Precipitates. Rozaliya Barabash, Gene Ice.

02:30-03:00 13.15.03
Study of the Local Distortions of RETe₃ (RE=rare earth) in the Charge-density-wave State using the Atomic Pair Distribution Function Analysis. H.J. Kim, E.S. Bozin, S.J.L. Billinge, C.D. Malliakas, M.G. Kanatzidis, Th. Proffen.

03:00-03:30 Coffee Break.

03:30-04:00 13.15.04
The Null-Matrix Method Applied to a NiPt Alloy. J.A. Rodriguez, S.C. Moss, J.L. Robertson, J.R.D. Copley, D.A. Neumann, J. Major.

04:00-04:30 13.15.05
X-ray Diffuse Scattering Study of Nano-scale Lattice Modulation in YBa₂Cu₃O_{7-x}. Xuerong Liu, Zahirul Islam, Sunil Sinha, Simon Moss, Jonathan Lang, Ulrich Welp.

04:30-05:00 13.15.06
Local Structure of Complex Phases of

NaNbO₃ by Neutron PDF. Daniel Mitchell, Wojciech Dmowski, Thomas Proffen, Takeshi Egami.

13.16 Time Resolved Scattering

P. Thiyagarajan, 301C
Vukica Srajer, Presiding

01:30-02:00 13.16.01
Structural Dynamics of Myoglobin Investigated by Time-resolved Laue Crystallography. Dominique Bourgeois.

02:00-02:30 13.16.02
Time Resolved Small Angle X-ray Scattering Study of Protein Folding. Satoshi Takahashi, Tsuyoshi Konuma, Yuji Goto, Tetsuro Fujisawa.

02:30-03:00 13.16.05
Time-Resolved Solution X-ray Scattering Studies on the Allosteric Transition of *E. coli* Aspartate Transcarbamoylase. Hiro Tsuruta, Jiarong Xia, Wenyue Guo, Elizabeth O'Day, Evan Kantrowitz.

03:00-03:30 Coffee Break.

03:30-04:00 13.16.04
The Z- to E- Isomerization in Biliproteins. Marius Schmidt, Anamika Patel, Wolfgang Reuter.

04:00-04:30 13.16.03
The Kinetics and Mechanisms of Pressure-Jump Induced Phase Transitions of Lyotropic Lipid Mesophases and Proteins. Roland Winter.

04:30-05:00 13.16.06
Sub-nanosecond Intermediate of PYP Photocycle Captured by Time-Resolved X-ray Crystallography. Hyotcherl Ihee, Yang Ouk Jung.

05:00-05:30 13.16.07
Time-Resolved Methods for Fiber Diffraction of Muscle. Tom Irving.

FRIDAY, JUNE 6	
2009 Toronto Meeting	
Planning Session	
08:30am	301A

2008 EXHIBIT SHOW

Saturday, May 31, 07:30pm-10:30pm

Show and Opening Reception

Monday, June 2, 10:00am-07:30pm

Show and Poster Session II

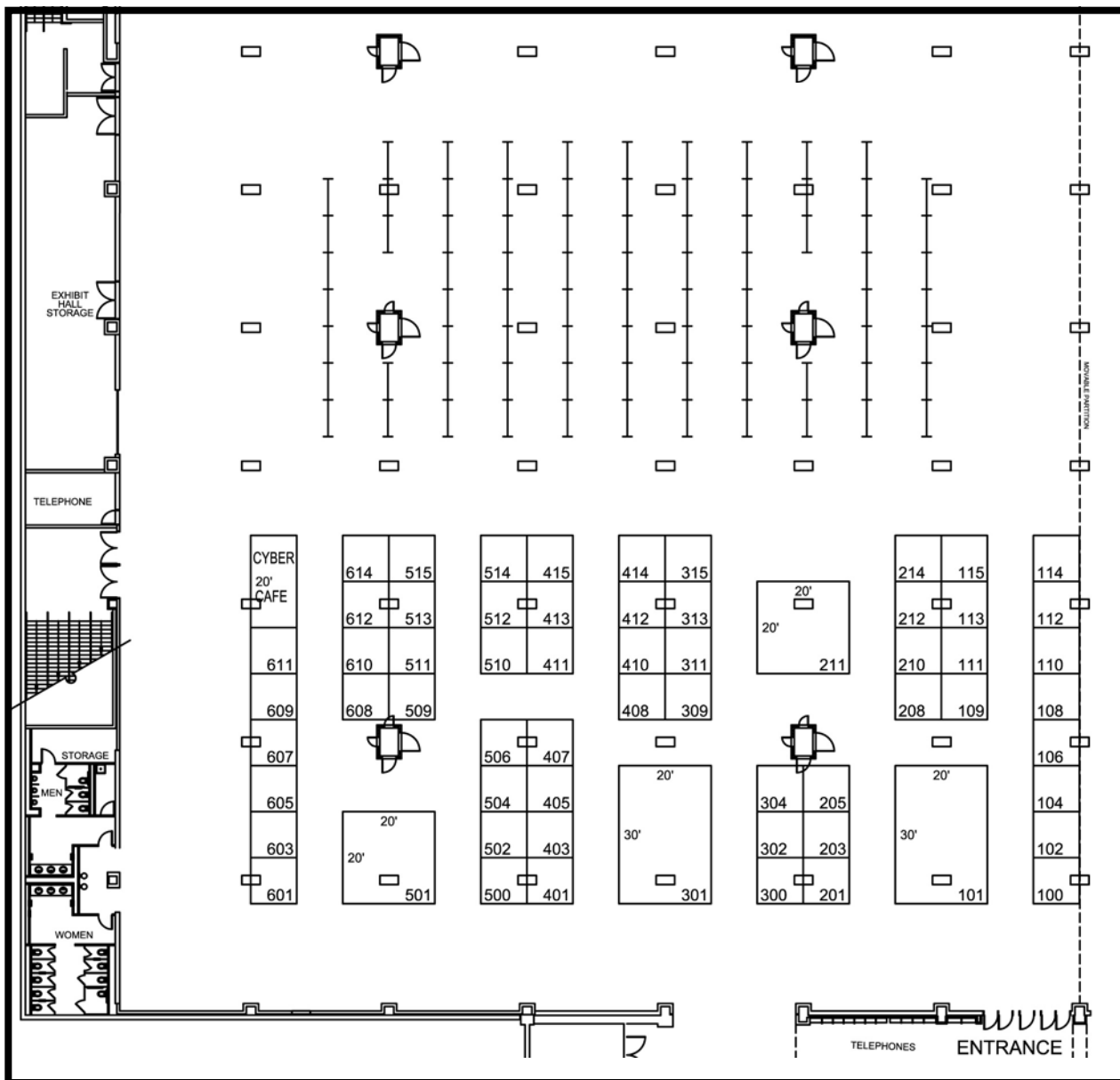
Sunday, June 1, 10:00am-06:30pm

Show and Poster Session I

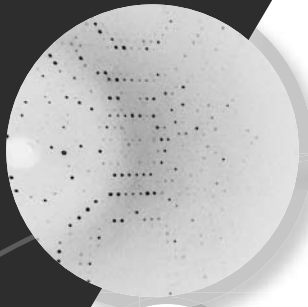
Tuesday, June 3, 10:00am-07:30pm

Show and Poster Session III

Anton Paar..... 115	Fluidigm Corp..... 208,210	Oxford Diffraction Inc..... 211
Area Detector Systems Corp 309,311	Formulatrix, Inc. 300,302	PANalytical 111
Art Robbins Instruments 100,102	GN Biosystems, Inc. 511	QIAGEN, Inc. 109
Axygen Biosciences 201	Greiner Bio-One 408	Rayonix, L.L.C. 411
Blake Industries, Inc. 214	Hampton Research 315	RCSB Protein Data Bank 500
BRANDEL 407	Incoatec GmbH 405	Rigaku 101
Bruker AXS Inc. 301	Korima Inc. 203	Southeast Regional Collaborative
CCP4 502	Marresearch GmbH..... 504	Access Team (SER-CAT) 506
Digilab Genomic Solutions..... 104,106	Mitegen, LLC 205	TTP Lab Tech Ltd..... 304
Douglas Instruments Ltd 513	Molecular Dimensions Inc..... 515	Wyatt Technology Corp. 401
ESRF - ILL..... 108,110	Oak Ridge National Lab 114	XENOCS SA 414
	Oxford Cryosystems..... 509	



Protein
Crystallography



Small Molecule
Crystallography



1 μ STM Incoatec Microfocus Source

30 W

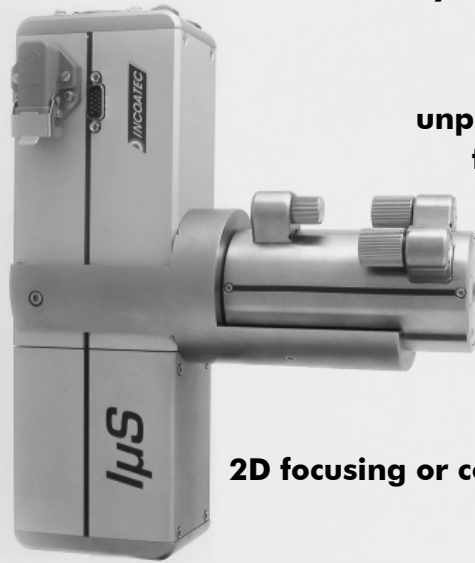
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flux density

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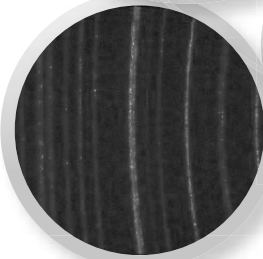
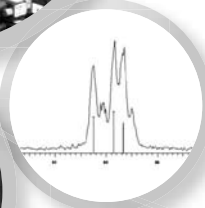


2D focusing or collimating

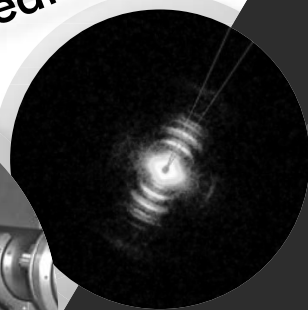
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SAXS



POSTERS

POSTER SESSIONS

Posters beginning with **S** will present in Poster Session I, on Sunday, June 1, 04:30pm - 06:30pm

Posters beginning with **M** will present in Poster Session II, on Monday, June 2, 05:30pm - 07:30pm

Posters beginning with **T** will present in Poster Session III, on Monday, June 3, 05:30pm - 07:30pm

All posters should be assembled before 04:30pm on Sunday and removed at the end of the poster session on Tuesday at 07:30pm. Please be present at your poster during the entire time on the day to which you are assigned.

MP001

The PSI Structural Genomics Knowledgebase. Helen M. Berman, Paul Adams, Andras Fiser, Adam Godzik, Andrei Kouranov, Rajesh Nair, Christine Orengo, Burkhard Rost, Wendy Tao, Torsten Schwede, Raship Shah, John Westbrook.

SP002

Crystal Structure of the Heterotrimer Core of the *S. cerevisiae* AMPK Homolog SNF1. Michael Rudolph, Gabe Amodeo, Liang Tong.

TP003

Formylglycinamide Ribonucleotide Amido-transferase from *Thermotoga maritima*: Structural Insights into the Complex Formation. Mariya Morar, Steven Ealick.

MP004

Instantly Identify Protein Crystals. G. Ra-vich, Vu Tran.

SP005

A Single-crystalline Photoreactive Cocrystal with a Rectangular Cross-section. Dejan-Kresimir Bucar, Leonard R. MacGillivray.

MP006

SAS Analysis in 2D and the DANSE project. Mathieu Doucet, Paul Butler.

TP007

Nitrile-Halogen Contacts in Benzylidene-anilines Revisited: The Influence of the Substitution Pattern. W.H. Ojala, K.M. Lystad, J.M. Spude, B.C. MacQueen.

SP008

A New Class of Organic Ligands Based on Cyclobutane: Design, Total Synthesis and Applications Thereof. Dejan-Kresimir Bucar, Quanli Chu, Phoung V. Dau, Stacy C. Sommerfeld, Claude L. Mertzenich, Leonard R. MacGillivray.

MP009

Molecular Basis of Passive Immunotherapy of Alzheimer's Disease. Chris Dealwis, Anna S. Gardberg.

TP010

The PXRR, a Resource for Macromolecular Crystallography at

NSLS. D.K. Schneider, A. Heroux, A.M. Orville, H.H. Robinson, A.M. Saxena, A. Soares, R.M. Sweet, L. Berman.

SP011

Racemic Polymorphs of 2-[Methyl(phenyl) amino]nicotinic Acid. Sihui Long, Sean Parkin, Maxime Siegler, Carolyn Brock, Tonglei Li.

TP012

Low Resolution SAXS Study of Human FEZ1: A Natively Unfolded Protein. Julio Cesar Silva, Daniel Lanza, Eliana Assmann, Alexandre Quaresma, Gustavo Bressan, Jorg Kobarg, Iris Torriani.

MP013

Applications of High Throughput Solution X-ray Scattering (SXS). Greg Hura, Michal Hammel, Robert Rambo, Shelley Claridge, Angeli Mennon, Paul Alivisatos, Mike Adams, John Tainer.

MP015

Determining the Telomere-Binding Properties of Glyceraldehyde-3-Phosphate Dehydrogenase (GAPDH). Neil Demarse, John Baatz, Eleanor Spicer, Besim Ogretmen, Christopher Davies.

SP016

New Protein Fold Revealed by a 1.65Å Resolution Crystal Structure of *Francisella tularensis* Pathogenicity Island Protein Iglc. Ping Sun, Brian Austin, Florian Schubot, David Waugh.

TP017

Structure of the Hypothetical Protein PF0899 from *Pyrococcus furiosus* at 1.85 Å Resolution. M. Gary Newton, L.L.C. Kelley, B. Dillard, W. Tempel, L. Chen, N. Shaw, D. Lee, F. Sugar, F. Jenney Jr., H.-S. Lee, C. Shaw, F. Poole, III, M. Adams, J. Richardson, D. Richardson, Z.-J. Liu, B.-C. Wang, J. Rose.

MP018

The Mode of Binding of Nitrogen Containing Bisphosphonates in Farnesyl Pyrophosphate Synthase. Bobby Barnett, James Dunford, Mark Lundy, X. Dao, Artem Evdokimov, Marlene Meckel, Richard Walter, X. Song, R. Boeckman, F. Ebetino.

TP019

SCrALS-Service Crystallography at the Advanced Light Source: A Collaborative Access Project for Chemical Crystallography. Jeanette Krause, Allen Oliver.

SP020

Temperature Induced Phase Transformations in Relaxor Ferroelectrics Lead Scandium Tantalate and Ba-doped Lead Scandium Tantalate. Bernd Maier, Boriana Mihailova, Carsten Paulmann, Thomas Malcherek, Joerg Ihringer, Martin Gospodinov, Rainer Stosch, Bernd Guettler, Ulrich Bismayer.

MP021

Structural Investigation of the Mechanism of Human Brain Aspartoacylase. Johanne Le Coq, Radhika Malik, Ronald Viola.

TP022

New Developments for Neutron and X-Ray Diffraction Studies at RT of Type III AntiFreeze Protein. Andre Mitschler, Matthew Blakeley, Isabelle Haertlein, Michael Haertlein, Christian Mueller-Dickmann, Alexander Popov, Eduardo Howard, Alberto Podjarny.

SP023

Surface Characterization of Uric Acid Crystals by Chemical Force Microscopy. Janeth Presores, Jennifer Swift.

TP024

Detergent-associated Solution Conformations of Membrane Proteins Studied by Small-angle X-ray Scattering. William Heller, Yiming Mo, Byung-Kwon Lee, Jeffrey Becker.

MP025

Independence of U2AF Activity on Interdomain Linker Composition. Jermaine Jenkins, Haihong Shen, Michael Green, Clara Kielkopf.

SP26

New Neutron Beamlines. C. Hoffmann.

MP027

Motion Control of the Iron-sulfur-protein in bcl Complex from *Rhodobacter sphaeroides*. Lothar Esser, Maria Elberry, Chang-An Yu, Linda Yu, Di Xia.

SP028

Altered Dimer Interface Decreases Stability in an Amyloidogenic Protein. James R. Thompson, Elizabeth M. Baden, Francis C. Peterson, Brian F. Volkman, Marina Alvarado-Ramirez.

TP029

Crystal Structure of Maltase-Glucoamylase as a Basis for Controlling Blood Glucose Levels. David R. Rose, Lyann Sim.

MP030

Micropatterned Flexible Crystallization Plates: Parameters and Applications. Robin Baur, Robert Thorne.

TP031

Design of Porous Solids from 2-D and 3-D Coordination Frameworks Utilizing Imidazolylbenzoic Acids. Lisa Lee, Yu Wang, John MacDonald.

MP033

Structural Impact of Three Parkinsonism-Associated Missense Mutations of Human DJ-1. Mark Wilson, Mahadevan Lakshminarasimhan, Marien Maldonado, Wenbo Zhou, Anthony Fink.

TP034

Design and Performance of the New Supermirror Guide on HRPD at ISIS. Richard Ibberson, K.S. Knight, L.C. Chapon, P.G. Rodaelli.

MP036

Transport Across the Bacterial Membrane: Structural and Functional Aspects of the Two Partner Secretion System. Vincent Villeret, Bernard Clantin.

SP037

Crystal Structure of the Human iNOS CaM-FMN Domain in Complex with Ca²⁺-Calmodulin. Chuanwu Xia, Ila Misra, Takashi Iyanagi, Jung-Ja P. Kim.

TP038

Structure-Function Studies of Enzymes Associated with Synthesis of Glycopeptide Antibiotics. Rong Shi, Sherry Lamb, Sathesh Bhat, Ariane Proteau, Traian Sulea, Gerard Wright, Allan Matte, Miroslaw Cygler.

MP039

SAXS, Lee-Richards Surfaces and a Simplified Command Set for Maps. Herbert J. Bernstein, Isaac Awuah Asiamah, Georgi Darakev, Nikolay Darakev, John Jemilawon, Nan Jia, Petko Kamburov, Greg McQuillan, Georgi Todorov.

SP040

Unusual Commonality and Phase Transformations within the Six Crystal Forms of an Active Pharmaceutical Ingredient. Michael Galella.

TP041

Modulation of Intensity in Neutron Spectroscopy. Markus Bleuel, Roland Gahler, Ed Lang, Jyotsana Lal.

MP042

Fragment-based Cocktail Crystallography Combined with *in silico* Chemical Screening to Target uracil-DNA Glycosylase of *Leishmania*. Eric Lar-son, W. Deng, S. Shibata, Z. Zhang, L. Xiao, N. Mueller, A. Napuli, W. Hol, C. Verlinde, E. Merritt, F. Zucker, F.S. Buckner, W.C.E. Van Vorhis.

MP044

Crystal Structure of Type II Restriction Endonuclease PabI Revealed Novel DNA Binding Fold and DNA-Recognition Mode. Kenichi Miyazono, Miki Watanabe, Jan Kosinski, Ken Ishikawa, Masayuki Kamo, Tatsuya Sawasaki, Janusz M. Bujnicki, Yaeta Endo, Masaru Tanokura, Ichizo Kobayashi, K. Nagata.

SP045

Crystal Structures of Human and *S. aureus* Pruvate Carboxylase and Molecular Insights into the Carboxyltransfer Reaction. Song Xiang, Tong Liang.

TP046

First Complex of Biphenyl Dioxygenase with a PCB: Crystal Structure of Biphenyl Dioxygenase with 2,6-Dichlorobiphenyl. Pravindra Kumar, L. Gomez-Gil, D. Bar-riault, M. Sylvestre, L.D. Eltis, J.T. Bolin.

MP047

An Electron Paramagnetic Resonance Study of the Jahn-Teller Effect in Copper Doped Cadmium-Histidine. Michael Colaneri, Jacqueline Vitali, Brenda Marmol.

SP048

Hydrogen Bonded Intercalation of Unsaturated Pyridyl into 1D-Coordination Polymers. Teresa Gonzalez, Alexander Briceo, Graciela Diaz de Delgado.

MP049

Studying Local Structural Aspects of Metal-Insulator Transition in Cu(Ir_{1-x}Crx)₂S₄ Using Total Scattering X-ray Atomic Pair Distribution Function. Emil Bozin, Ahmad Masadeh, Hyun Jeong Kim, Pavol Juhas, John Mitchell, Simon Billinge.

TP050

Combined Charge-Density, Time-Resolved Photocrystallographic and Theoretical Study of the Properties of K₂MVPtop. Milan Gembicky, Katarina Matuszna, Mateusz Pitak, Marc Messerschmidt, Philip Coppens.

MP052

Targeting DNA Replicative Proteins from Hyperthermophilic and Psychrophilic Archaea for Structure Determination. M.L. Byrne, R.C. Hughes, D. Marsic, E.J. Meehan, J.D. Ng.

TP053

Homodimeric Structure and dsRNA Cleavage Activity of the C-terminal RNase III Domain of Human Dicer. Daijiro Takeshita, Shuhei Zenno, Kaoru Saigo, Masaru Tanokura.

MP054

Using RasMol, PyMol and Jmol with the Structural Biology Extensible Visualization Scripting Language (SBEVSL). Paul A. Craig, Scott E. Mottarella, Corey Wischmeyer, Herbert J. Bernstein, Isaac Awuah Asiamah, Darina Boycheva, Georgi Darakev, Nikolay Darakev, Philip Gozo, John Jamilawon.

TP055

New Opportunities for Powder Diffraction at SNS. Ashfia Huq, Jason Hodges.

SP056

A Magic Triangle? Experimental Phasing of Macromolecules with a Triiodo Benzene Derivative. Tobias Beck, George Sheldrick.

MP057

Structure of Protein MMP1218 from *Methanococcus maripaludis* S2. Norma Duke, Brittany Conrad, Rory Mulligan, Minyi Gu, Andrzej Joachimiak.

SP058

Structure and Function of Achaean Enzyme 5-Formaminoimidazole-4-carboxamide-1-β-D-ribofuranosyl 5'-Monophosphate Synthetase. Yang Zhang, Robert H. White, Steven E. Ealick.

TP059

Structural and Mutational Studies of Anthocyanin Malonyltransferases Establish the Features of BAHD Enzyme Catalysis. Hideaki Unno, Fumiko Ichimaida, Hirokazu Suzuki, Seiji Takahashi, Yoshikazu Tanaka, Atsushi Saito, Tokuzo Nishino, Masami Kusunoki, Toru Nakayama.

- MP060
Adventures in Chirality. Frank Fronczek.
- TP061
Nondispersive Kirkpatrick-Baez Neutron Supermirror Optics. Gene Ice, Chris Tulk, Jamie Molaison, Peter Takacs, Ken Andersen, Thierry Bigault.
- SP062
Structural Basis for the Iron Uptake Mechanism of *Helicobacter pylori* Ferritin. Ki Joon Cho, Ji-Hye Lee, Hye Jeong Shin, In Seok Yang, Seung Taik Lim, Kyung Hyun Kim.
- TP065
A Cobalt Beacon in the Active Site of Human Carbonic Anhydrase II. Balendu Avvaru, Daniel Arenas, Chingkuang Tu, David Tanner, Mavis Agbandje-McKenna, David Silverman, Robert McKenna.
- MP066
pKa Predictions of Turkey Ovomuroid Third Domain via a New CHARMM Based Generalized Born Algorithm: A Validation Study Comparing Experimental Versus Predicted. Francisco Hernandez-Guzman, Velin Spassov.
- TP067
A High-field (30-45 Tesla) Pulsed Magnet Instrument for X-ray Studies of Materials at the Advanced Photon Source. Zahirul Islam, Jacob Ruff, Yasuhiro Matsuda, Zhe Qu, Hiroyuki Nojiri, Shunsuke Yoshii, Bruce Gaulin, Zhiqiang Mao, Jonathan Lang.
- SP068
Structure of the *Nitrosomonas europaea* Rh Protein. Xin Li, Sanjay Jayachandran, Hiep-Hoa Nguyen, Michael Chan.
- MP069
Structural Studies on Vitamin B₆ Catabolism. Kathryn McCulloch, Tathagata Mukherjee, Tadhg Begley, Steven Ealick.
- TP070
Structural Studies of Type IIE Restriction Endonuclease *EcoRII*-DNA Complexes. Liqing Chen, Li Qiu, Michal Szczepek, Monika Reuter, Edward J. Meehan.
- SP071
The Crystal Structure of SARS nsp9 G104E. Zachary Miknis, Timothy Umland, L. Wayne Schultz.
- MP072
A Neutron Sensitive Anger Camera for Neutron Scattering Instruments. John Richards, Ronald Cooper, Theodore Visscher, Cornelius Donahue.
- TP073
Polysaccharide Structures: A Heuristic Journey from Laboratory Source to Synchrotron Radiation. Srinivas Janaswamy, Ren-gaswami Chandrasekaran.
- SP074
High Resolution Crystal Structures of the HIV-1 Protease and the I54V Mutant Reveal Tetrahedral Reaction Intermediates. Yunfeng Tie, Andrey Kovalevsky, Alexander Chumanovich, Chen-Hsiang Shen, John Louis, Robert Harrison, Irene Weber.
- TP075
Toward a Joint X-ray/Neutron Refinement of the Cysteine Peptidase Papain: The Room Temperature X-ray Structure. Anna Gardberg, Hugh O'Neill, Edward Snell, Dean Myles.
- SP076
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- TP077
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- MP078
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- SP079
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- MP080
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- TP081
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- MP082
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- MP085
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- TP086
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- MP087
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- TP088
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- TP090
Crystal Structure of Human Checkpoint Kinase 2 in Complex with a Potent & Selective Inhibitor. George Lountos, Andrew Jobson, Joseph Tropea, Di Zhang, Robert Shoemaker, Yves Pommier, David Waugh.
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A Simulation Study of Scattering from Molecular Models with Random Physical Variations, Applied to Protein Models Derived from SAXS Data. Stefan Sillau, Mark van der Woerd, Jay Breidt.

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Magnetic Annealing Effects on Local Atomic Environment in Fe₂₀Ni₈₀. Yevgeniy Puzyrev, Gene Ice, Paul Zschack.

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Crystal Structure of Trioxacarcin A Covalently Bound to DNA. Roland Pfoh, George Sheldrick.

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Crystal Structures of Different Inhibited and Redox Forms of Cytochrome *c* Oxidase Show Changes in Proton Pathways. Ling Qin, Jian Liu, Martyn A. Sharpe, Denise A. Mills, Carrie Hiser, R. Michael Garavito, Shelagh Ferguson-Miller.

MP099

Phase Equilibria and Crystal Chemistry of the BaO-Nb₂O₅ and BaO-WO₃-Nb₂O₅ Systems. Claudia Rawn, W. Brandon Goodwin, Antonio dos Santos, Joseph Muth.

SP100

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

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Allosteric Regulation in the Bacterial GTPase BipA Revealed Through Structural and Biochemical Studies. Victoria L. Robinson, Raymond S. Brown, Tobias P. Neef, Megan A. deLivron.

MP102

Wavelength-Shifting Fiber Scintillation Neutron Detectors for POWGEN3 & VULCAN at SNS. Lowell Crow.

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The Crystal Structure of the siRNA Binding Domain of an Argonaute Protein from the Novel Hyperthermophilic Archaeon *Thermococcus thio-reducens*. Ronny C. Hughes, Miranda L. Byrne, Joseph D. Ng.

TP105

The Structural and Kinetic Implications of Glu 106 Mutations on Proton Shuttling in Human Carbonic Anhydrase II. Katherine Sippel, Jeanne Quirit, A. Savoy, Chingkuang Tu, John Domsic, David Silverman, Mavis Agbandje-McKenna, Robert McKenna.

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Crystal Structure of the Isolated IQGAP1 GAP-related Domain. Vinodh Kurella, Courtney Bryan, Jessica Ricks, Henry Bellamy, David Worthylake.

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The Crystal Structures of *Enterococcus* Aminoglycoside (2") Phosphotransferase Variants Ib and Ic, Enzymes Implicated in Antibiotic Resistance. Clyde Smith, Paul Young, Laura Byrnes, Ted Baker.

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Magnetic Structural Changes of Cobalt Oxide under High Pressure. Antonio dos Santos, Christopher Tulk, Jaime Molaison, Bryan Chakoumakos.

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Crystal Structure of Conserved Domains of *Streptococcus mutans* Adhesion Protein Antigen I/II Reveals a Polyproline-type II Helix Interacting with an Extended α -helix. Matt Larson, Kanagalghatta Rajashankar, Lawrence Delucas, Suzanne Michalek, Jeannine Brady, Champion Deivanayagam.

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Crystal Structure of an RNA Methyltransferase in Complex with RNA and S-adenosylhomocysteine. Chao Tu, Joseph Tropea, Brian Austin, David Waugh, Donald Court, Xinhua Ji.

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Time-of-Flight Neutron Crystallography at the Protein Crystallography Station at Los Alamos National Laboratory. S. Zoe Fisher, Andrey Kovalevsky, Marat Mustyakimov, Mary Jo Waltman, Benno Schoenborn, Paul Langan.

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The Crystal Structure of TTHA0415, a Putative ACP Reductase from *Thermus thermophilus* at 1.9 Å Resolution. James Tucker Swindell II, L. Chen, A. Ebihara, A. Shinkai, S. Kuramitsu, S. Yokoyama, Z.-Q. Fu, J. Chrzas, J. P. Rose, B. C. Wang.

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A Key Metabolic Enzyme as an Attractive Target for Antibiotic Development. Ronald Viola, Xuying Liu, Alexander Pavlovsky, Chris Faehnle.

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Development of a Compact Crystal Positioning System for the TOPAZ Single Crystal Diffractometer at the Spallation Neutron Source. Matthew Frost, Christina Hoffmann, Michael Austin, Peter Carmen, Echo Miller, Lisa Mosier, Robert Viola.

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An Open and Flexible Robotic System Designed Towards Autonomous Protein Crystal Harvesting. Robert Viola, Peter Carmen, Jace Walsh, Echo Miller, Mark Balas, Cameron Wright, Bernhard Rupp.

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The Structure of a DnaB-Family Replicative Helicase and its Interactions With Primase. Ganggang Wang, Michael Klein, Etienne Tokonzaba, Yi Zhang, Lauren Holden, Xiaojiang Chen.

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Structure of the Catalytic Trimer of *Methanococcus jannaschii* Aspartate Transcarbamoylase in an Orthorhombic Crystal Form. Jacqueline Vitali, Michael Colaneri.

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MP128

A High Pressure Diffractometer at the Spallation Neutron Source. Jamie Molaison, Christopher Tulk, Antonio Moreira dos Santos, Gene Ice.

SP129

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TP130

X-ray Crystal Structures of N-semiquinone and Iminoquinone Forms of *Hansenula polymorpha* Copper Amine Oxidase. Carrie Wilmot, Bryan Johnson, Peder Cedervall, Brandon Goblirsch, Judith Klinman.

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The Effect of Homopolymer on the Morphology and Domain Size of Diblock Copolymer/Nanoparticle Complexes in a Selective Solvent. Vilas Pol, Chieh-Tsung Lo, Byeongdu Lee, R. Winans, P. Thiagarajan.

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Optimization of Inhibitors of the Human Cytoplasmic Protein Tyrosine Phosphatase. Kristoff T. Homan, Deepa Balasubramaniam, Olaf Wiest, Paul Helquist, Cynthia V. Stauffacher.

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The Molecular Basis of MAP Kinase Regulation by HePTP. David Critton, Breann Brown, Antoni Tortajada, Rebecca Page.

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An Automated Pipeline for Doing Molecular Replacement Including Search Model Discovery and Preparation. Ronan Keegan, Martyn Winn, Peter Briggs, Wanjuan Yang.

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New Opportunities for Simple Access to Automated Crystal Handling at the NSLS. Alexei Soares, Mary Carlucci-Dayton, Howard Robinson, Robert Sweet, Dieter Schneider.

SP138

The Role of the Dimeric Interface in the Catalytic Mechanism of Human Manganese Superoxide Dismutase. John Domsic, Jiayin Zheng, Patrick Quint, Diane Cabelli, David Silverman, Robert McKenna.

TP139

Refinement with Local Structure Similarity Restraints (LSSR) Enables Exploitation of Information from Related Structures and Facilitates use of NCS. Oliver Smart, Maria Brandl, Claus Flensburg, Peter Keller, Wlodek Paciorek, Clemens Vornrhein, Gerard Bricogne, T.O. Womack.

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SAXSess - An Analytical Tool for Nanostructured Biomaterials. P. Kotnik, H. Schnablegger, O. Glatter, Ch. Moitzi.

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Crystal Structure of *Streptococcus pneumoniae* Nicotinamidase with Bound Inhibitor Provides Insight into Mechanism of Catalysis. Jarrod French, Anthony Sauve, Steven Ealick.

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CCP4 Diffraction Image C++ Library. Francois Remacle, Graeme Winter.

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Small-Angle Neutron Scattering of Microemulsion Systems Containing pH-Degradable Surfactants for Protein Encapsulation and Drug Delivery. Douglas Hayes, Javier Gomez del Rio, Volker Urban, J.S. Lin.

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A Study of Protocatechuate 3,4-dioxygenase Mutants and Substrate Interactions. Rebecca Hoelt, Ke Shi, Zu-Yi Gu, C. Kent Brown, Jeff Digre, Cathleen A. Earhart, Douglas H. Ohlendorf.

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Reconstruction of Molecular Envelopes by SAXS has Implications for Molecular Modeling of APOBEC3G and the APOBEC-1 Complementation Factor (ACF). Jason Salter, Jolanta Krucinska, Ryan Bennett, Chad Galloway, Richard Gillilan, Harold Smith, Joseph Wedekind.

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Structural Insights into Substrate Specificity in Copper Amine Oxidases from *Hansenula polymorpha*. Valerie Klema, Cindy Chang, Bryan Johnson, Minae Mure, Judith Klinman, Carrie Wilmot.

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A More Automated Approach to Data Collection for Macromolecular Crystallography. Billy Poon, Peter Zwart, Paul Adams, Nicholas Sauter.

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Preliminary Neutron and Ultrahigh Resolution X-ray Single Crystal Diffraction Studies of the Aspartic Proteinase Endothiapepsin Co-crystallized with a Gem-diol Inhibitor PD-135,040. Han-Fang Tuan, Leighton Coates.

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Distant Homology Detection Using a Length and Structure-based Sequence Alignment Tool (LESTAT). Marianne Lee, Ralf Bundschuh, Michael Chan.

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Influence of Matrix Block Copolymer Structure on the Dynamics of Domain-specific Nanoparticles. David Bohnsack, Vilas Pol, Byeongdu Lee, Alec Sandy, Randall Winans, Pappannan Thiagarajan.

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A 1.6 Å Resolution Crystal Structure of cis-3-Chloroacrylic Acid Dehalogenase Reveals an Additional Active Site Residue - R117. Youzhong Guo, Hector Serrano, William Johnson, Christian Whitman, Marvin Hackert.

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A Rasmol to PyMOL Translator. Scott Mottarella, Brett Hanson, Charles Westin, Paul Craig, Herbert Bernstein.

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16 K Synchrotron X-ray Charge Density Study of Coordination Polymer, $\text{Co}_3(\text{C}_8\text{H}_4\text{O}_4)_4(\text{C}_4\text{H}_{12}\text{N})_2(\text{C}_5\text{H}_{11}\text{NO})_3$ at ChemMast CARS, APS. Y.S. Chen, H.F. Clausen, J. Overgaard, B.B. Iversen.

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Desktop Minstrel UV™: A Novel Protein Crystal Monitoring Automation System Using UV Fluorescence Microscopy. Jian Xu, Craig Sterling, Michael Willis.

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Time-of-Flight Neutron Diffraction Study of Human Deoxyhemoglobin. Andrey Kovalevsky, Toshiyuki Chatake, Takuya Ishikawa, Naoya Shibayama, Sam-Yong Park, Marat Mustyakimov, Paul Langan, Yukio Morimoto.

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New Macromolecular Crystallography Beam Line Facilities at the Stanford Synchrotron Radiation Laboratory. Herbert Axelrod, Clyde Smith.

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BioCARS: A State-of-the-art Facility for Time-resolved Crystallography with 100ps Time Resolution. Robert Henning, Timothy Graber, Vukica Srajer, Yu-Sheng

Chen, Zhong Ren, Friedrich Schotte, Phillip Anfinrud, Keith Moffat.

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Time-resolved Macromolecular Crystallography at BioCARS, Sector 14. Advanced Photon Source. V. Srajer, T. Graber, R. Henning, S. Ruan, Z. Ren, Y.-S. Chen, K. Moffat, P. Anfinrud, F. Schotte, W.E. Royer, J. Knapp.

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Enhanced Micro-Diffraction Capabilities at GM/CA CAT. Venugopalan Nagarajan, Mark Hilgart, Sudhir Babu Pothineni, Shenglan Xu, Sergey Stepanov, Michael Becker, Oleg Makarov, Ruslan Sanishvilli, Craig Ogata, Robert Fischetti.

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Structure of Bacterial Multiheme Cytochromes at the Microbial-mineral Interface. Alexander Johs, Wang Wei, Baohua Gu, John F. Ankner, Dean A. Myles, Liyuan Liang.

Poster Prizes

Pauling

The Pauling Poster Prize was established by the ACA, and is supported by member contributions, to honor Linus Pauling. Linus Pauling was one of the pioneers in American structural research and was very supportive



of the ACA. At each annual meeting the five best student (graduate or undergraduate) poster presentations receive Pauling awards. In addition, one poster is selected as the IUCr winner. The Larry Calvert CNC/IUCr Trust Fund sponsors a prize from a poster from Canadian laboratory. Winners will be notified before the banquet on Wednesday, June 4.



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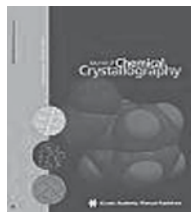
The Oxford Cryosystems Low Temperature Poster Prize is awarded to the best poster describing work in low temperature crystallography. The winner will receive a cash prize donated by Oxford Cryosystems, Inc. The winner will be announced at the banquet on Wednesday, June 4.



RCSB Protein Data Bank

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

The Journal of Chemical Crystallography



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

book voucher. The winner will be announced at the banquet on Wednesday, June 4.

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Axygen Biosciences offers a unique and complete **Custom Screens** and **Reagent Crystallography Service**. It will provide you with freedom to design and order **your own** Initial or Follow Up Screens and Reagents or to order Axygen-designed Initial or Follow Up Screens and Reagents. Here are the choices you have:

- A. Initial Screens designed by Axygen or designed by **you**
- B. Follow up kits based on Axygen's Initial Screens preliminary results
- C. Custom Follow up/Optimization Screens designed by **you**
- D. Custom Follow up or Optimization Screens designed by Axygen
- E. Axygen's Crystallography Reagents (Ready to use Buffers, Precipitants, Salts, Additives, and Detergents)
- F. Your own Crystallography Reagents

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