

2009 NIGMS Workshop – Enabling Technologies for Structural Biology
March 4-6, 2009
Natcher Conference Center, NIH

DRAFT

Wednesday, March 4

7:15 am Registration, Refreshments and Poster Setup

7:55 am Opening Remarks – **John Norvell** and **Jeremy Berg**

Session I Protein-Protein Interactions and Complexes

Chair: **Celia Goulding**

8:00 am Keynote Lecture, **Professor Michael Rossmann**, Purdue University, The Limits Of Crystallography Mark The Beginnings Of Biology: Structural Studies Of Viral Pathogens

8:50 am **Cliff Qiangfeng Zhang**, Structural Alignment In Predicting Protein-Protein Interaction

9:15 am **Li-Chung Ma**, Structural Biology of Influenza Viruses – Applications of Technologies from Structural Genomics

9:40 am **20 minute** Coffee Break and Poster Viewing

Session II Promoted Talks

Chair: **Celia Goulding**

10:00 am **Carthene Bazemore-Walker**, Identification of Sigma-1 Receptor Post-translational Modifications and Interacting Proteins Using Chemical Proteomics

10:25 am **Qiang Wang**, MOLIDE2: Homology Modeling Of Protein Oligomers And Complexes

10:50 am **Marc Deller**, Structural Dissection Of The Pentose Phosphate Pathway Of *Thermotoga Maritima*

11:15 am **Mariam Konate**, Skyline as a Discovery Tool for Phosphoinositide-Binding Proteins

11:40 am **Lunch**

Session I & II speakers at Designated Tables in Cafeteria
Session III & IV speakers in Designated Tables in Cafeteria

Open Poster Session

1:00 pm – 7:00 pm

Session III Promoted Talks

Chair: **Geoff Waldo**

- 1:00 pm **Igor Jurisica**, PSI Target Prioritization, Cancer Target Selection And Interpretation Using Protein-Protein Interaction Prediction And Analysis
- 1:25 pm **Barry Honig**, TBD
- 1:50 pm **Lee Makowski**, Characterizing The Unsolved Proteins Of The PSI Using WAXS
- 2:15 pm **M. Gordon Joyce**, A Rational Approach for Heavy Atom Derivatization of Macromolecules
- 2:40 pm **Yao Fan**, Enhanced Crystal Packing Due To Solvent Reorganization Through Reductive Methylation
- 3:05 pm **25 minute** Coffee Break and Poster Viewing

Session IVa Pedagogical Talks on Structure Methods

Chair: **Michael Malkowski**

- 3:30 pm **High-Throughput Crystallization Screening and Optimization; Deriving Information to Guide Successive Experiments**, presented by Joseph R Luft, Edward H Snell, Jennifer L Wolfley, Raymond M Nagel, Christina K Veach, Angela M Lauricella, Eleanor L Cook, M Elizabeth Snell, Max H Thayer, Stephen A Potter, Michael M Malkowski & George T DeTitta.
- The Microcapillary Protein Crystallization System (MPCS): A Methods Tutorial**, presented by Cory Gerdts, Peter Nollert, Rustem Ismagilov & Lance Stewart.
- Semi-Automatic Structure Solution with HKL-3000**, presented by W Minor, M Cymborowski, Z Otwinowski & D Borek.
- The Center For High-Throughput Structural Biology – Crystallographic Data Collection Facilities At SSRL**, presented by A. E. Cohen, S. M. Soltis & the SMB group at SSRL.

Session IVb Pedagogical Talks on Structural Analysis

Chair: **Helen Berman**

- 3:30 pm **How to Use the Protein Structure Initiative Structural Genomics Knowledgebase for Research**, presented by Margaret J Gabanyi, John D Westbrook, Wendy Tao, Raship Shah, Andrei Kouranov, & Helen M. Berman.
- Getting the Most from Your Structure**, presented by Adam Godzik, Sri Krishna & Constantina Bakolitsa,
- 5:30 pm **Session IV Close**

Standby Poster Session

5:30 pm Authors of odd-numbered posters standby
6:15 pm Authors of even-numbered posters standby
7:00 pm **Poster Session Close**

Conference Dinner

7:30 pm Bethesda area restaurant to be named

Thursday, March 5

7:15 am **Refreshments and Poster Viewing**

Session V Protein Function

Chair: **Brian Fox**

8:00 am Keynote Lecture, **Professor Frank Raushel**, Texas A&M University,
Deciphering Substrate Specificity of Enzymes of Unknown Function

8:50 am **Markus Fischer**, MarkUs: A Function Annotation Server For Protein Structures
9:15 am **Tonya Silkov**, Structural Characterization And Functional Annotation Of The
Novel Families Of Membrane-Binding Proteins

9:40 am **20 minute** Coffee Break and Poster Viewing

Session VI Promoted Talks

Chair: **Brian Fox**

10:00 am **T. Andrew Binkowski**, Protein Surface Analysis For Function Analysis And
Prediction

10:25 am **David Aceti**, A “Control Workgroup” Of 24 Protein Targets Used To Test
Platform Changes

10:50 am **Ying Zhang**, Metabolic Docking—from Structural Genomics to Functional
Genomics

11:15 am **Brian Chen**, Relating Volumetric Similarity To Substrate Specificity

11:40 am **Lunch**

Session V and VI speakers at Designated Tables in Cafeteria
Session VII and VIII speakers in Designated Tables in Cafeteria

Open Poster Session

1:00 pm – 7:00 pm

Session VII Promoted Talks

Chair: **Ashley Deacon**

- 1:00 pm **Geoffrey S. Waldo**, Fluorescent Protein Toolbox: Application To Structural Genomics And Cell Biology
- 1:25 pm **Stephen Anderson**, Extra-Cellular Mammalian Proteins As Structural Genomics Targets
- 1:50 pm **Mark Knuth**, Application Of Medium Scale Robotics For Eukaryotic Cell Expression, Purification, And Analysis To PSI Targets
- 2:15 pm **Vadim Cherezov**, New LCP Technologies for Structural Studies of Membrane Proteins
- 2:40 pm **Robert Thorne**, Slow Cooling For Protein Cryocrystallography
- 3:05 pm **25 minute** Coffee break and Poster Viewing

Session VIa Pedagogical Talks on High-throughput Purification

Chair: **Celia Goulding**

- 3:30 pm **Semi-Automated High Throughput Protein Purification for Structural Biology**, presented by YC Kim, I Dementieva, R Wu, P Quartey, L Volkart, C Hatzos, N Maltseva, L Bigelow, R Mulligan, E Duggan, M Borovilos, A Sather, C Tesar, R Hendrick, H Li, M Zhou & A. Joachimiak.
- Improving Protein Crystallization using Protein Reductive Methylation**, presented by YC Kim, P Quartey, L Volkart, C Hatzos, CS Chang, B Nocek, M Cuff, J Osipiuk, K Tan, Y Fan, L Bigelow, N Maltseva, R Wu, M Borovilos, E Duggan, H Li, M Zhou, A Binkowski, RG Zhang & A. Joachimiak.
- Simple Methods for Monitoring Protein State and Protein Sample Composition by NMR and Light Scattering Measurements**, presented by Innokentiy Maslennikov, Georgia Kefala, Chris Dickson, Senyon Choe & Witek Kwiatkowski.

Session VIb Pedagogical Talks on Expression of Proteins

Chair: **Brian Fox**

- 3:30 pm **Hands-on Demonstration of Wheat Germ Cell-free Translation**, presented by Shin-Ichi Makino, Michael A Goren, Brian G. Fox, Kazuyuki Takai, Hidenori Hayashi, John L. Markley & Yaeta Endo.
- Cell-free Expression of Integral Membrane Proteins**, presented by Christian Klammt, Innokentiy Masennikov, Witek Kwiatkowski & Senyon Choe.
- Condensed Single Protein Production (cSPP) of Isotope-Enriched Soluble and Membrane Proteins for Structural Studies**, presented by Masayori Inouye and Gaetano Montelione.
- 5:30 pm **Session Close**

Standby Poster Session

5:30 pm Authors of odd-numbered posters standby
6:15 pm Authors of even-numbered posters standby
7:00 pm **Poster Session Close**

Friday, March 6

7:15 am **Refreshments and Poster Viewing**

Session VIII Promoted Talks

Chair: **Gaetano Montelione**

8:00 am **Thomas Szyperski**, Compiling And Sharing Experience In Research Networks Using 'Wikis' – An Approach For The NESG NMR Section
8:25 pm **Antonio Rosato**, The eNMR Platform For Structural Biology
8:50 am **Yuanpeng Huang**, HTP Construct Optimization using Bioinformatics Coupled with an Amide Hydrogen Deuterium Exchange (HDX) and HTP NMR Screening
9:15 am **Chad Rienstra**, Protein Structure Determination By Magic-Angle Spinning NMR
9:40 am **Srivatsan Raman**, Predicting Protein Structures to Atomic-Level Accuracy Using Limited NMR Data

10:05 am **20 minute** Coffee Break and Poster Take-Down

10:25 am **Steven Almo**, Atoms To Animals: Structural And Functional Genomics Of Immunity
10:50 am **Kemin Tan**, The Structure and Function of α -Glucosidase from Human Gut Bacterium *Ruminococcus obeum*
11:15 am **Bart Staker**, Ligand Screening At The Seattle Structural Genomics Center For Infectious Disease (SSGCID)
11:40 am **John Hunt**, Towards Structurally Enabled High-Throughput Function Elucidation

12:05 pm **Closing Statements**

12:20 pm **Lunch** – Organizers final meeting