

ISGO International Conference on Structural Genomics Berlin, 10 – 13 October 2002

Program (with late changes)

Thursday, 10 October 2002

- 10.00 – 15.00** **Registration**
- 10.00 – 13.30** ***Open ISGO Structural Genomics Task Force Meetings***
(Chair: Tom Terwilliger)
- 10.00 – 10.15 *Udo Heinemann (Berlin, Germany)*
Brief introduction into structural genomics, the ISGO, and the structural genomics task forces
- 10.15 – 10.30 *Tom Terwilliger (Los Alamos, NM, USA)*
Task force on numerical criteria for evaluating and assuring structure quality
- 10.30 – 10.45 *Steve Bryant (Bethesda, MD, USA)*
Task force on tracking and registration of targets
- 10.45 – 11.00 *Helen Berman (Piscataway, NJ, USA)*
Task force on deposition, archiving, and curation of the primary information
- 11.00 – 11.15 *Guy Dodson (York, UK)*
Task force on mechanisms for publication and recording of methods
- 11.15 – 11.35** ***Break***
- 11.35 – 11.50 *Barbara Skene (London, UK) and John Norvell (Bethesda, MD, USA)*
Task force on intellectual property and data release
- 11.50 – 12.35 *Lawrence Sung (Baltimore, MD, USA)*
Impact of patent rights on the dissemination and use of structural genomic data
- 12.35 – 13.30 *Open discussion about ISGO and ISGO task forces*
- 15.00 – 15.20** **Welcome**
Representatives of
the Max Delbrück Center for Molecular Medicine,
the Berlin senate,
the Federal Ministry for Education and Research,
and the International Structural Genomics Organisation (ISGO)
- 15.20 – 16.20** **Opening Lecture** (Chair: Udo Heinemann)
Robert Huber (Martinsried, Germany)
Molecular machines for protein degradation

- 16.20 – 17.00** **Plenary Lecture** (Chair: Dave Stuart)
Chris Dobson (Cambridge, UK)
Protein folding and its links to the evolution of protein structure
- 17.00 – 18.00** **Protein Production for Structural Genomics**
(Chair: Shigeyuki Yokoyama)
- 17.00 – 17.20 Dave Stuart (Oxford, UK)
Piecing together the Oxford pipeline
- 17.20 – 17.40 Naomi Chayen (London, UK)
Tackling the bottleneck of protein crystallization for structural genomics
- 17.40 – 17.50 Takanori Kigawa (Yokohama, Japan)
High-throughput screening of proteins suitable for structure determination: Overview
- 17.50 – 18.00 Geoffrey S. Waldo (Los Alamos, NM, USA)
Engineering proteins for high-throughput structural genomics
- 18.00 – 21.00** **Welcome Mixer and Poster Session 1 (Including Mega Posters)**
- 19.00 – 19.30** ***Finissage zu Ausstellung & Projekt CROSSING OVER (Foyer MDC.C)***
Karsten K. Panzer (PerZan)

Friday, 11 October 2002

- 09.00 – 09.40** **Plenary Lecture** (Chair: Hartmut Oschkinat)
Kurt Wüthrich (Zürich/San Diego)
NMR in structural and functional genomics
- 09.40 – 10.40** **Membrane Proteins** (Chair: Kurt Wüthrich)
- 09.40 – 10.00 Lars-Oliver Essen (Marburg, Germany)
Halorhodopsin: Light-driven ion pumping made simple?
- 10.00 – 10.20 Timothy A. Cross (Tallahassee, FL, USA)
Integral membrane proteins structural genomics: *Mycobacterium tuberculosis*
- 10.20 – 10.40 César Fernández Estrabao (Zürich, Switzerland)
Solution NMR structure of the *E. coli* outer membrane protein OmpX
- 10.40 – 11.10** **Coffee Break**
- 11.10 – 11.50** **Plenary Lecture** (Chair: Ivano Bertini)
Chris Sander (Cambridge, USA)
The challenge of structural genomics

- 11.50 – 12.50** **Structural Genomics and Disease** (Chair: Ian Wilson)
- 11.50 – 12.10 Wim Hol (Seattle, WA, USA)
Medicinal protein crystallography and structural genomics for tropical diseases
- 12.10 – 12.30 Duncan McRee (San Diego, CA, USA)
A high-throughput protein crystallography pipeline for structure-based drug design
- 12.30 – 12.50 Ditlev Brodersen (Cambridge, UK)
Binding of antibiotics to the 30S ribosomal subunit
- 12.50 – 15.00** **Lunch Break and Poster Session 1 (Including Mega Posters)**
- 13.30 – 14.40** ***Perspectives for Structural Genomics in Europe***
(Room: Dendrite II/III)
(Chair: Udo Heinemann)
- 13.30 – 13.50 *Dave Stuart (Oxford, UK)*
Structural genomics in Europe: Slow start, strong finish?
- 13.50 – 14.10 *Josefina Enfedaque (European Commission, Brussels)*
Structuring European research in structural genomics
- 14.10 – 14.40 *Open discussion*
- 15.00 – 15.40** **Plenary Lecture** (Chair: Sung-Hou Kim)
- Dino Moras (Illkirch, France)
Ligand binding to nuclear hormone receptors
- 15.40 – 16.20** **Biological Insight from Large Sets of Protein Structures**
(Chair: Sung-Hou Kim)
- 15.40 – 16.00 Sarah Teichmann (Cambridge, UK)
Domain duplications and combinations in *Escherichia coli* metabolic enzymes
- 16.00 – 16.20 Jeff Bonanno (New York, NY, USA)
The GHMP kinase superfamily: Evolutionary and mechanistic implications arising from structural studies
- 16.20 – 16.50** **Coffee Break**
- 16.50 – 17.50** **Verified Hypotheses from Protein Structures**
(Chair: Andrzej Joachimiak)
- 16.50 – 17.10 Sung-Hou Kim (Berkeley, CA, USA)
Molecular functions of "hypothetical proteins" inferrable by their structures
- 17.10 – 17.30 Aled Edwards (Toronto, Canada)
Biochemical validation of structural hypotheses
- 17.30 – 17.50 Hartmut Oschkinat (Berlin, Germany)
Hypotheses about activities and functions of non-catalytic protein domains from NMR investigations

- 17.50 – 19.10** **NMR Methods for Structural Genomics** (Chair: Cheryl Arrowsmith)
- 17.50 – 18.10 Miguel Llinás (Pittsburgh, PA, USA)
Is it NMR or is it crystallography? CLOUDS, a direct method for protein structure elucidation via NMR proton densities.
- 18.10 – 18.30 Gaetano Montelione (Piscataway, NJ, USA)
Automated analysis of protein NMR assignments and structures
- 18.30 – 18.50 Peter Güntert (Yokohama, Japan)
Automated NMR structure calculation with the new software CYANA
- 18.50 – 19.10 Michael A. Kennedy (Richland, WA, USA)
NMR-based structural genomics at the Pacific Northwest National Laboratory, USA
- 20.00** **Speakers' Dinner** (by invitation)

Saturday, 12 October 2002

- 09.00 – 09.40** **Plenary Lecture** (Chair: Samar S. Hasnain)
Janet L. Thornton (London, UK)
From protein structure to biological function
- 09.40 – 10.40** **Bioinformatics: Protein Space** (Chair: Chris Sander)
- 09.40 – 10.00 Nicholas O'Toole (Montreal, Canada)
Analysis of worldwide structural genomics targets
- 10.00 – 10.20 Sung-Hou Kim (Berkeley, CA, USA)
A global view of the protein fold space
- 10.20 – 10.40 Liisa Holm (Helsinki, Finland)
More for less in structural genomics
- 10.40 – 11.10** **Coffee Break**
- 11.10 – 12.10** **Functional Genomics** (Chair: Gaetano T. Montelione)
- 11.10 – 11.30 Marc Vidal (Cambridge, MA, USA)
Toward a proteome atlas for *C. elegans*
- 11.30 – 11.50 Stefan Wiemann (Heidelberg, Germany)
Large-scale subcellular localisation and functional analysis of novel proteins
- 11.50 – 12.10 Steven Brenner (Berkeley, CA, USA)
Alternative splicing, protein structure, and gene regulation

- 12.10 – 13.10** **Hot Topics** (Chair: B.C. Wang)
- 12.10 – 12.30 Gu Xiaocheng (Beijing, China) with Shi Yunyu, Liwen Niu, Zihao Rao,
and Hai Pang
Structural genomics effort in China
- 12.30 – 12.50 Bill Studier (Brookhaven, NY, USA)
Protein production with inducible T7 expression systems
- 12.50 – 13.10 Allampura M. Babu (Berlin, Germany)
Design of web book to handle meta-crystallographic data
- 13.10 – 15.00** **Lunch Break and Poster Session 2**
- 13.20 – 14.40** **Commercial Session (Room: Dendrite II/III)**
(Chair: Patrick Umbach)
- 13.20 – 13.50 Erhard Fernholz (Roche Biosciences, Penzberg, Germany)
Using cell-free protein expression systems by Roche RTS technology
- 13.50 – 14.15 Dietrich Carlhoff (Amersham Biosciences, Uppsala, Sweden)
Automation of multidimensional protein chromatography
- 14.15 – 14.40 Günther Knebel (Greiner BioOne, Frickenhausen, Germany)
High throughput vapor diffusion and microbatch protein crystallization
- 15.00 – 15.40** **Plenary Lecture** (Chair: Wolfram Saenger)
- Wayne A. Hendrickson (New York, USA)
Structural genomics of histidine kinase sensors
- 15.40 – 16.40** **Bioinformatics: Function** (Chair: Chris Sander)
- 15.40 – 16.00 Olivier Lichtarge (Houston, TX, USA)
An accurate, scalable method to identify functional sites in protein
structures
- 16.00 – 16.20 Kengo Kinoshita (Yokohama, Japan)
Analysis of complementarity of protein-DNA interactions using the
molecular surface database, eF-site
- 16.20 – 16.40 Takanori Tanaka (Yokohama, Japan)
Characteristics and prediction of domain linker sequences in multi-
domain proteins
- 16.40 – 17.10** **Coffee Break**

- 17.10 – 18.30** **X-ray Methods for Structural Genomics**
(Chair: Tom C. Terwilliger)
- 17.10 – 17.30 Victor Lamzin (Hamburg, Germany)
ARP/wARP for automated modelling and refinement of protein crystal structures: the next generation
- 17.30 – 17.50 Tom C. Terwilliger (Los Alamos, NM, USA)
Automated structure solution, density modification, and model building for MAD, SAD and MIR
- 17.50 – 18.10 Wayne F. Anderson (Chicago, IL, USA)
Automating crystallographic structure determination
- 18.10 – 18.30 Dominika Borek (Dallas, TX, USA)
Phasing protocols for structural genomics
- 20.00** **Conference Dinner**

Sunday, 13 October 2002

- 10.00 – 11.00** **International Coordination for Structural Genomics**
(Chair: Tom C. Terwilliger)
- 10.00 – 10.20 Helen Berman (Piscataway, NJ, USA)
Enabling high-throughput data deposition to the Protein Data Bank
- 10.20 – 10.40 Mitch Guss (Sydney, Australia)
Facilitating publication of the results from structural genomics efforts
- 10.40 – 11.00 Tom C. Terwilliger (Los Alamos, NM, USA)
ISGO -- International cooperation in structural genomics
- 11.00 – 11.30** **Coffee Break**
- 11.30 – 12.10** **Plenary Lecture** (Chair: Klaus Peter Hofmann)
Shigeyuki Yokoyama (Yokohama, Japan)
Structural genomics and proteomics of genetic and cell signaling systems
- 12.10 – 13.10** **Protein Production for Structural Genomics, continued**
(Chair: Shigeyuki Yokoyama)
- 12.10 – 12.30 Christine Lang (Berlin, Germany)
A micro-scale process for high-throughput expression of cDNAs in the yeast *Saccharomyces cerevisiae*
- 12.30 – 12.50 Alexei Savchenko (Toronto, Canada)
Strategies for rapid and efficient production of structural proteomics samples
- 12.50 – 13.10 Andrzej Joachimiak (Argonne, IL, USA)
Automation of protein purification for structural genomics

- 13.10 – 15.00** **Lunch Break and Poster Session 2**
- 15.00 – 15.40** **Plenary Lecture** (Chair: Matthias Wilmanns)
Stephen K. Burley (San Diego, USA)
Structure-based drug discovery
- 15.40 – 16.40** **Applications from Protein Structures**
(Chair: Wayne A. Hendrickson)
- 15.40 – 16.00 Yoonsang Cho (College Station, TX, USA)
Crystal structure of ATP phosphoribosyltransferase from
Mycobacterium tuberculosis: a potential TB drug target
- 16.00 – 16.20 Chantal Abergel (Marseille, France)
In search for new anti-bacterial target genes: a comparative/structural
genomics approach
- 16.20 – 16.40 Larissa Podust (Nashville, TN, USA)
Structural genomics of the cytochrome P450 superfamily from
Streptomyces: applications for generating new antibiotics
- 16.40** **Close of Conference**