

# PDB40

## Symposium

October 28-30, 2011

Cold Spring Harbor Laboratory  
Grace Auditorium

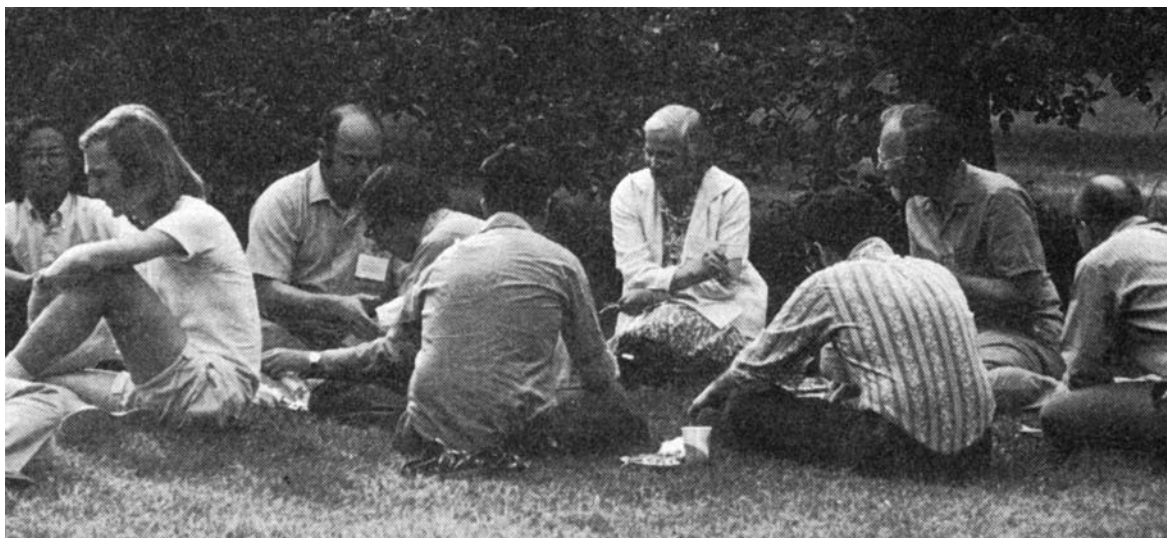
PROGRAM



## About PDB40

This symposium, which marks the 40<sup>th</sup> anniversary of the Protein Data Bank (PDB), celebrates the field of structural biology and the continued growth and development of the PDB.

In June 1971, a symposium on *Structure and Function of Proteins at the Three Dimensional Level* was held at Cold Spring Harbor Laboratory (CSHL).



*Photo courtesy CSHL*

With its lively conversations, debates, and planning for the future, that meeting defined the beginning of the PDB as an archive for the experimentally determined 3D structures of biological macromolecules.

The Worldwide Protein Data Bank (wwPDB) has returned to CSHL to commemorate the event and to inspire conversations and collaborations that will help guide the PDB for the next 40 years.

PDB40 has been organized by: Helen M. Berman (RCSB PDB), Gerard Kleywegt (PDBe), Haruki Nakamura (PDBj), John Markley (BMRB), and Stephen K. Burley (wwPDB Advisory Committee and Eli Lilly & Company).

*The organizers would like to thank the PDB40 speakers, Cold Spring Harbor Laboratory, the many sponsors listed in this program, and PDB staff past and present who have all made an impact on this important resource.*

# Conference Program

**Friday, October 28**

5:30 p.m.      *Reception*                      *Racker Room/Blackford Hall*  
6:30 p.m.      *Dinner*                                      *Blackford Hall/Main Dining Room*

**Session I**                      **Chair: Helen Berman** (Rutgers University)                      *Grace Auditorium*

8:15 p.m.      **Michael Rossmann**                      The PDB: A historical perspective  
*Purdue University*

9:00 p.m.      **Stephen K. Burley**                      Growth, globalization, and future  
*Eli Lilly & Company*                      of the PDB

9:45 p.m.      *Posters & Light Refreshments*      *Grace Lobby*

*We encourage everyone to visit the posters throughout the meeting.  
Posters will be on display from the opening reception to the closing lunch.*

# Conference Program

**Saturday, October 29**

7:30 a.m.      *Breakfast*      *Blackford Hall/Main Dining Room*

**Session II**      **Chair: Joel Sussman** (Weizmann Institute of Science)      Grace Auditorium

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9:00 a.m.      **Janet Thornton**  
*EMBL-European  
Bioinformatics Institute*      Abstracting knowledge from protein structures for biology in the 21<sup>st</sup> century

9:30 a.m.      **David Baker**  
*University of Washington*      Scientific discovery by protein folding game players

10:00 a.m.      **Andrej Sali**  
*University of California,  
San Francisco*      Determining architectures of macromolecular assemblies by aligning interaction networks to electron microscopy density maps

10:30 a.m.      *Break*      *Refreshments in Grace Lobby*

**Session III**      **Chair: Phil Bourne** (University of California, San Diego)      Grace Auditorium

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11:00 a.m.      **Jane Richardson**  
*Duke University Medical Center*      Studying and polishing the PDB's macromolecules

11:30 a.m.      **Ad Bax**  
*National Institute of Diabetes &  
Digestive & Kidney Diseases/NIH*      An NMR view of the interaction between viral fusion proteins and phospholipids

12:00 p.m.      **Axel Brunger**  
*Stanford University/HHMI*      Challenges for structure determination at low resolution

12:30 p.m.      *Lunch*      *Blackford Hall/Main Dining Room*

# Conference Program

**Saturday, October 29 cont.**

**Session IV**      **Chair: Tom Koetzle** (Brookhaven National Laboratory, retired)      Grace Auditorium

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- 2:00 p.m.      **Cheryl Arrowsmith**      Structural and chemical biology of the  
*University of Toronto*      readers and writers of the histone code
- 2:25 p.m.      **Susan Taylor**      Evolution of protein kinases: Insights from  
*University of California, San Diego*      the structural kinome
- 2:50 p.m.      **Soichi Wakatsuki**      Coevolution of synchrotron radiation  
*KEK Photon Factory and*      crystallography  
*Structural Biology Research Center*
- 3:15 p.m.      *Break*      *Refreshments/Grace Lobby*

**Session V**      **Chair: Haruki Nakamura** (Osaka University)      Grace Auditorium

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- 3:45 p.m.      **Richard Henderson**      What is needed to make single particle  
*MRC Laboratory of*      electron cryomicroscopy reach its  
*Molecular Biology*      true potential?
- 4:10 p.m.      **Wah Chiu**      CryoEM of molecular machines  
*Baylor College of Medicine*
- 4:35 p.m.      **Angela Gronenborn**      Synergy between NMR and CryoEM:  
*University of Pittsburgh*      Novel findings for HIV capsid function
- 5:00 p.m.      *Posters & Cocktails*      *Grace Lobby/Patio*
- 6:30 p.m.      *Dinner*      *Blackford Hall/Main Dining Room*

**Session VI**      **Chair: Gerard Klewegt** (EMBL-EBI)      Blackford Hall/Main Dining Room

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- 8:30 p.m.      **Johann Deisenhofer**      Remarks  
*UT Southwestern Medical Center*

# Conference Program

**Sunday, October 30**

7:30 a.m. *Breakfast* *Blackford Hall Main Dining Room*

**Session VII** **Chair: John Markley** (University of Wisconsin-Madison) *Grace Auditorium*

9:00 a.m. **Kurt Wüthrich** *The Scripps Research Institute/  
ETH Zürich* Structural biology by NMR and the Protein Data Bank

9:30 a.m. **Mei Hong** *Iowa State University* Membrane protein solid-state NMR: Elucidating the influenza M2 structure and mechanism

10:00 a.m. *Break* *Refreshments in Grace Lobby*

**Session VIII** **Chair: Gary Gilliland** (Centocor R&D, Inc.) *Grace Auditorium*

10:30 a.m. **David Searls** *Independent Consultant* Macromolecular linguistics

11:00 a.m. **Wayne Hendrickson** *Columbia University* SLAC1 and the splendor of atomic resolution

11:30 a.m. **Helen Berman** *Rutgers University* Closing Remarks

12:30 p.m. *Lunch* *Blackford Hall/Main Dining Room*

**Departures**

## Interactive Displays

Please join us in reminiscing about the PDB's past and imagining its future.

### Historical Displays

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Cold Spring Harbor Laboratory has organized a display of pictures from the 1971 meeting, and another that highlights the history of the crystallography course called *X-ray Methods in Structural Biology* that has been held on campus since 1988.

While many of the people pictured from the 1971 meeting have been identified, some have not. Please help us update the CSHL archives by writing down the names of people you recognize in the space provided at the display.

### What will the PDB look like in 10 years? In 40?

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While the establishment of an archive to freely share and exchange scientific data was visionary in 1971, it would have been challenging to predict what the PDB would look like at its 40<sup>th</sup> anniversary.

The PDB has grown immensely in the past 40 years. Many of the structures and technologies commonplace in structural biology today were unimaginable in 1971.

What are your visions for the future? How will the Protein Data Bank evolve over the next decade? Where will we be for PDB80?

Please write down your predictions and add them to the PDB poster board.

## Poster Presentations

Poster abstracts are available online at <http://meetings.cshl.edu/meetings/pdb40.shtml>.

\* denotes travel award recipient

Poster #	Author	Poster title
1*	Hiromi Arai	Crystal structure of a conformation-dependent rabbit IgG Fab fragment specific for a sequence-independent generic epitope associated with prefibrillar amyloid oligomers
2*	Ryoichi Arai	Domain-swapped dimeric structure of a <i>de novo</i> 4-helix bundle protein, WA20
3*	Pelin Armutlu	A TOG: $\alpha\beta$ -tubulin complex structure suggests conformation-based mechanisms for a microtubule polymerase
4	Christopher Bahl	The <i>Pseudomonas</i> virulence factor Cif alters human ABC transporter trafficking and stability through epoxide hydrolase enzyme activity
5	Ramanuj Banerjee	Threaded dimer assembly of the novel Psu fold from Enterobacteria phage P4
6*	Avraham Ben-Shimon	Deciphering the arginine-binding preferences of Ser/Thr kinases by computational surface mapping
7	Talapady Bhat	Managing 2D and 3D ligand fragments from PDB and PubChem
8	Shveta Bisht	<i>Escherichia coli</i> Diaminopropionate ammonia lyase–Structure, substrate specificity and catalysis
9*	Spencer Bliven	A comprehensive comparison of protein structures and the correlation of structure with function
10	Matthias Buck	Dynamic protein-protein complexes–How alternative interactions create ensembles and how solution NMR and MD simulations can characterize them
11	Brianne Burkinshaw	Salmonella virulence protein SopB down-regulates activity of host Rho GTPase Cdc42 by mimicking a nucleotide dissociation inhibitor
12*	Arindam Chakrabarty	Unique crystal structure of protozoan parasite <i>Entamoeba histolytica</i> malic enzyme
13*	Tammy Cheng	Structural biology meets systems biology–Gauging the systemic impact of single nucleotide polymorphisms
14*	Alvaro Cortes	AtlasCBS–A web server to graphically represent the content of chemico-biological databases
15	Charles Dann III	Treatment of cancer and autoinflammatory disease for over sixty years–Structural basis for folate and antifolate trafficking via human folate receptors
16*	Teresa De la Mora	Crystal structures of eIF4E in complex with Bn <sup>7</sup> -GMP
17*	Bryan Der	Metal-mediated affinity and orientation specificity in a computationally designed protein homodimer
18	Jianping Ding	Regulation of the histone acetyltransferase activity of hMOF via autoacetylation of Lys274
19	Wolfgang Dostmann	A structural analysis of the regulatory domain from the cGMP-dependent protein kinase I $\alpha$
20	Joseph Dybas	Evolution of protein structures from the perspective of their super-secondary structure building blocks
21*	Clarissa Eibl	Crystal structure of NLRP4 pyrin domain

Poster #	Author	Poster title
22	Richard Feldmann	The second log
23	Javier Fernandez-Martinez	Structure-function Map of a heptameric module in the nuclear pore complex
24	Barry Finzel	The use of distance geometry for substructure searching and local superposition in DNA, RNA, and protein-polynucleotide complexes
25	Andras Fiser	Predicting protein structure with supersecondary-structure building blocks and basic NMR data
26*	Szu-Chin Fu	Prediction of leucine-rich nuclear export signal containing proteins with NESsential
27*	Kyoko Furuita	NMR structural studies of the complex between lipid binding protein OSBP and ER membrane protein VAP-A
28	Miwako Homma	Autophosphorylation of CK2 $\alpha$ at the N-terminal region is required for its catalytic activity
29*	Corey Hryc	Hybrid de novo modeling for 4 Å resolution cryo-EM maps of viruses
30	Valentin Ilyin	PFAT-Protein Functional Annotation based on TOPOFIT
31	Valentin Ilyin	N-TOPOFIT-DB, a DNA / RNA 3-D structural alignment database by N-TOPOFIT
32	Hitoshi Inada	Structure of human TRPV4 ankyrin repeat domain
33	Constance Jeffery	Moonlighting proteins
34*	Fangling Ji	Solution NMR and biophysical analysis of the cataract-associated R76S mutant of human $\gamma$ D-crystallin
35	Holly Jing	Discovery of novel inhibitors of therapeutic targets using fragment-based lead discovery methods
36	Jan Johansson	Prevention of amyloid $\beta$ -peptide fibrillation-Insights from the BRICHOS domain structure
37	Chisa Kamada	Supercomputational life science in Japan
38	Tatsuki Kashiwagi	Crystallization of proteins in high magnetic force fields aiming at high resolution structures
39	Takeshi Kawabata	Chemical similarity-based docking to receptor proteins by searching maximum common substructure
40	Choel Kim	Structural and biochemical studies of the cGMP selectivity for cGMP dependent protein kinase
41*	Seung Joong Kim	Integrative structure determination of the components of the nuclear pore complex by X-ray crystallography, small angle X-Ray scattering, electron microscopy, NMR and comparative modeling
42*	Serah Kimani	Unexpected reactions resulting from mutating catalytic residues in an amidase reveal the role of the catalytic unit
43*	Yu Kitago	Structural basis for peptide ligand recognition by LR11 Vps10p domain
44	Stefan Knight	Structural basis for control of spider silk assembly-A conserved N-terminal solubility relay
45	Adrian Laurenzi	Improving EST annotation with protein structure prediction software
46	Tali Lavy	The GAL regulon in <i>S. cerevisiae</i> -The Gal3p/Gal80p interaction

Poster #	Author	Poster title
47	Thomas Leeper	Silver (I) metallated protein structures derived by combined NMR and X-ray crystallographic analyses
48	Yang Lei	A maximum-likelihood approach to local real-space model fitting
49*	Alejandra Leo-Macias	In vitro reconstituted F-actin and fascin bundles studied by cryoelectron tomography and subtomogram averaging
50*	Yunfeng Li	Crystal structure and functional studies of the GerBC component of a <i>Bacillus subtilis</i> spore germination receptor
51*	Vidya Mangala Prasad	Towards a structure for the Rubella virus capsid protein
52	Manish Manish	Computational design of conformationally intact immunogen for the elicitation of protective antibody immune response
53	Stefano M. Marino	Extreme evolutionary pressure determines Cysteine residues distribution in protein molecular surfaces
54	Yamuna Kalyani Mathiwaran	Domain swapping and protein symmetry–Investigations on the stationary phase survival protein SurE as a model
55	William McLaughlin	A searchable set of predictions of protein functions with associated probabilities as derived from annotations of protein sequences and three-dimensional structures
56	Wenli Meng	Unfolded proteins can form long range contacts under strongly denaturing conditions in the absence of significant secondary structure
57	Thomas Moon	Autoinhibition and salt sensing are linked in the WNK1 kinase
58	Andrew Morin	The SBGrid Consortium–Enabling structurally biology computation
59*	Chie Motono	SAHG, a comprehensive database of predicted structures of all human proteins
60*	Kensuke Nakamura	Structural analysis of BAR domain of Arfaptin in complex with small GTPase Arl1
61	Janet Newman	Getting better at crystallisation by learning from the past
62*	Ilona Nudelman	Observation of intermolecular interactions in large protein complexes by 2D-double difference NOESY–Application to the 44 kDa interferon-receptor complex
63	Åsa Nylander	Structural studies of streptococcal adhesins
64	Sang Ho Park	Computational docking studies of histone deacetylase 8 (HDAC8) and its inhibitors by AutoDock Vina program
65*	Aviv Paz	Sugar transport inhibition of the sodium galactose transporter
66	Janez Plavec	NMR solution-state structures of monomeric and dimeric G-quadruplexes adopted by a sequence from N-myc
67*	Pavel Plevka	Mechanism of re-organization of flavivirus glycoproteins during maturation
68	Mario Pujato	The evolution of robustness involves balancing of local sequence and network architecture level mechanisms
69	Pavlina Rezacova	Crystal structures of the effector-binding domain of repressor CggR from <i>Bacillus subtilis</i> reveal ligand-induced structural changes upon binding of several glycolytic intermediates
70	Florian Richter	A computational method to design backbone conformations featuring predefined interactions

Poster #	Author	Poster title
71	Victoria Robinson	Elucidating the mechanism of action of the translation factor BipA
72	Aleksandr Sahakyan	Protein structures from the perspective of side-chain chemical shifts
73	Stefan Schoebel	LidA from Legionella is a Rab-supereffector
74*	Masaaki Shiina	X-ray crystallographic analysis of Runx1-CBF $\beta$ -Ets1-DNA complex assembled on the enhancer of T cell receptor $\alpha$ chain gene
75	Irena Sieglova	Structure of the effector-binding domain of arabinose repressor AraR from <i>Bacillus subtilis</i>
76*	Peter Stranges	Accurate design of a symmetric homodimer using $\beta$ -strand assembly
77	Juergen Suehnel	The Jena Library of Biological Macromolecules-JenaLib
78	Juergen Suehnel	The Jena3D viewer for visualization of biological macromolecules
79*	Hiroshi Sugimoto	Structure and catalytic mechanism of iron-dependent enzymes
80*	Mitsuhiro Takeda	Recent progress in a stereo-array isotope labeling (SAIL) method for NMR structure determination
81	Todd Taylor	Discriminating thermophilic proteins from their mesophilic analogs
82	Eldon Ulrich	The Biological Magnetic Resonance Data Bank (BMRB)
83	Ihsanawati Wahab	Structural basis for the high alkaliphily of modular xylanase XynJ from <i>Bacillus</i> sp. 41M-1
84	Gary Wesenberg	The role of peptide-peptide stacking interactions in protein structure
85	Carrie Wilmot	In crystallo synthesis of the tryptophan tryptophylquinone cofactor of methylamine dehydrogenase
86*	Mousheng Wu	Structural basis of the Ca <sup>2+</sup> inhibitory mechanism of <i>Drosophila</i> Na <sup>+</sup> /Ca <sup>2+</sup> exchanger CALX and its modification by alternative splicing
87*	Guozhou Xu	Structure, substrate specificity and mechanism of kinase activation of the I $\kappa$ B kinase $\beta$ (IKK $\beta$ )
88*	Yusuke Yamada	Automation of data collection and processing at the Photon Factory macromolecular crystallography beamlines
89	Olga Yuzlenko	Membrane protein native state discrimination by a physical energy function
90	Huan Zhan	Influence of membrane dipole potential on peptide binding to lipid bilayers
91	Yan Zhang	Dephosphorylation regulation of RNA polymerase II in eukaryotic transcription
92	Yong Zhang	From NMR information to high accuracy biomolecular structures-A quantum chemical pathway
93*	Samira Zouhir	Structural study of a molecular switch implicated in quorum sensing in <i>Bacillus cereus</i>

# Meeting Information

## Campus Map



### Wireless

Cold Spring Harbor Laboratory has wired and/or wireless access throughout much of campus. Cabins have wireless access only. Wireless internet access is available in Grace Auditorium, Lobby and environs; Blackford Dining Hall and Racker Reading Room. Computers and printers are available on main and lower levels of Grace Auditorium.

### Audio-Visual Facilities

The audio-visual team is located in the office in the rear of Grace Auditorium and maintains a projection suite of state of the art audio and visual technologies run by both Mac and PC. Presenters are asked to download their talks onto our presentation computers before their sessions.

### Photography

A roving photographer, Connie Brukin, will be taking photos during the conference. These photos will be posted after the meeting at [meetings.cshl.edu/galleries/galleries.html](http://meetings.cshl.edu/galleries/galleries.html)

A group photograph will be taken of everyone present who has worked for the PDB since its inception. Please listen for announcements made during the breaks.

### Departures

On Sunday, CSHL will be providing a shuttle service to the train station.

Syosset Limo (516 364-9681) will offer bus rides to JFK and LaGuardia airports for \$45. Buses will depart at 1:00 p.m. and 3:00 p.m. Please sign up for this service on the bulletin board provided.

Travel arrangements can also be made with Syosset Taxi (516 921-2141).

# Sponsors

The organizers would like to thank the following sponsors for their support of PDB40:

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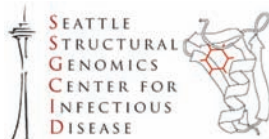


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## Meeting Host



Cold Spring Harbor Laboratory