RCSB PDB NEWSLETTER

NUMBER 23 FALL 2004 *Published quarterly by the Research Collaboratory for Structural Bioinformatics Protein Data Bank*

Weekly RCSB PDB news is available on the Web at www.rcsb.org/pdb/latest_news.html

Links to RCSB PDB newsletters are available at www.rcsb.org/pdb/newsletter.html

Contents

Snapshot: October 1, 2004

27,428 released atomic coordinate entries

Molecule Type		Experimental Technique	
24,882	proteins, peptides, and viruses	23,435	diffraction and other
1,358	nucleic acids	14,133	structure factor files
1,170	protein/nucleic acid complexes	3,993	NMR
18	carbohydrates	2,069	NMR restraint files

Participating RCSB Members

Rutgers: rutgers.rcsb.org

SDSC/UCSD: www.pdb.org

CARB/UMBI/NIST: nist.rcsb.org

E-mail: info@rcsb.org

FTP: ftp.rcsb.org

The RCSB PDB is a member of the wwPDB (www.wwpdb.org)

Message from the RCSB PDB

The RCSB PDB attended a variety of meetings this past quarter to demonstrate the use of RCSB tools (such as pdb_extract for structure deposition) and the reengineered RCSB PDB site and database (which is still undergoing beta testing at pdbbeta.rcsb.org).

Special events at these meetings were also organized by the RCSB:

• Together with CCP4, a session aimed at depositors entitled "A Protein Crystallographic Toolbox: CCP4 Software Suite and RCSB PDB Deposition Tools" was held at the American Crystallographic Association's Annual Meeting (ACA; July 17-22; Chicago, IL). Presentations including "An Introduction to the CCP4 Software Suite", "pdb_extract and CCP4: Making Deposition Easier", and "Validation and Deposition at the RCSB Protein Data Bank" can be downloaded from CCP4 (**www.ccp4.ac.uk**). Also at the ACA meeting, RCSB PDB, CCP4, and CCDC formed a "Data Alley" with these groups next to each other in the exhibition hall.

Some members from RCSB and CCP4 at "A Protein Crystallographic Toolbox: CCP4 Software Suite and RCSB PDB Deposition Tools"

• On September 10, the "Database Challenges in Biology" symposium at CARB brought together experts in biological data management to describe how data are organized to enable scientists to derive new knowledge about structure and function. Special thanks goes to the speakers at this event, who are highlighted in the Related Links shown on page 7.

This newsletter looks at other presentations from this quarter, including the 3D SIG and ISMB/ECCB meeting and a report on the workshop for high school students and teachers "X-rays, Molecules, and You".

The RCSB PDB

Data Deposition and Processing

5 Steps for Crystal Structure Deposition

At the ACA meeting, annotator Kyle Burkhardt presented a poster entitled "Deposition and Annotation at the RCSB PDB". This poster described 5 steps for depositing crystal structures:

1. Use the pdb_extract Program Suite (available on the Web and as a software download)

2. Check your structure with the PDB Validation Suite (available on the Web and as a software download)

3. Run BLAST (at NCBI - **www.ncbi.nlm.nih.gov/BLAST**)

4. Use Ligand Depot to identify and define your ligands

5. Deposit your structure using ADIT (available on the Web at RCSB-US, PDBj, and as a software download)

A brochure that summarizes this poster is available from **deposit.pdb.org/xtal-struct-dep.pdf**. These steps utilize RCSB PDB data deposition tools available from **deposit.pdb.org/depoinfo/depotools.html**.

PDB Focus: How Are HPUB Structures Released?

The release status of a structure is determined by the author at the time of deposition. The status HPUB is used to indicate that a structure will be released when the corresponding journal article is published. Publication is considered to be when the article is distributed by the publisher, either in print or electronically. The RCSB emails the depositor to either confirm that the publication corresponds to the structure, or to indicate that the structure will be released because the article includes the PDB ID.

The RCSB PDB receives publication dates and citation information from some journals. For other journals, the RCSB PDB scans the literature for publication information. We also greatly appreciate the citation information that is sent to us at deposit@rcsb.rutgers.edu from the community.

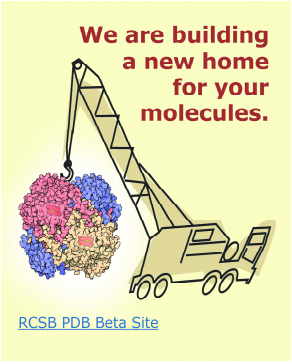
PDB Deposition Statistics

As of October 1, approximately 4128 structures have been deposited in the PDB archive in 2004. Of the structures received, 77% were deposited with a "hold until publication" release status; 13% with a "release immediately" status; and 10% with a specific release date.

83% of these entries were the result of X-ray crystallographic experiments; 14% were determined by NMR methods.

Data Query, Reporting, and Access

RCSB PDB Beta Site



As announced in the Summer 2004 newsletter, the RCSB PDB Beta Site (**pdbbeta.rcsb.org**) is a completely reengineered system using more consistent and comprehensive data from the data uniformity project. Data are integrated with sequence, function and disease related information and are available by browsing and searching.

The RCSB is very excited about this resource, and encourages the PDB community to test the new site. We look forward to feedback sent to **betafeedback@rcsb.org**.

RCSB PDB Presentations and Demonstrations at 3D SIG/ISMB/ECCB and the Protein Society Meeting

The 2004 Intelligent Systems for Molecular Biology (ISMB) conference (July 31-August 4; Glasgow, Scotland) was combined this year with the European Conference on Computational Biology (ECCB). With over 2100 attendees, this was the largest gathering of computational biologists ever. The meeting was preceded by 3D SIG (July 29-30), the first special interest group meeting on structural bioinformatics.

The RCSB PDB gave several software demonstrations of the RCSB PDB Beta Site at 3D SIG and ISMB. Wolfgang F. Bluhm also presented a poster on this new site.

Another poster, "Protein Data Bank - Current State and Proposed Transition to a Re-engineered Query System," was presented at the 18th Symposium of the Protein Society (August 14-18, 2004, San Diego Marriot Hotel) by Nita Desphande.

Website Statistics

The RCSB PDB is available from several Web and FTP sites located around the world. Users are also invited to preview the newly reengineered RCSB website at **pdbbeta.rcsb.org**.

The access statistics are given below for the primary RCSB PDB website at **www.pdb.org**.

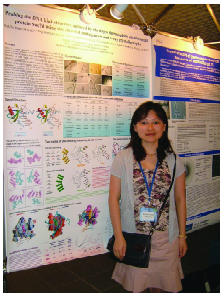
Access Statistics for **www.pdb.org**

	DAILY AVERAGE		MONTHLY TOTALS			
MONTH	HITS	FILES	SITES	KBYTES	FILES	HITS
Jul 04	202,250	149,975	84,185	193,063,880	4,499,252	6,067,522
Aug 04	189,558	142,549	78,904	195,736,236	4,276,497	5,686,761
Sep 04	278,806	202,946	112,025	247,205,987	5,885,455	8,085,402

RCSB Poster Prize Awarded at AsCA, ACA, and ECM

Thanks to the students and judges who participated in the RCSB Poster Prize competitions during this past quarter. The prize is designed to recognize student poster presentations involving macromolecular crystallography. The award was *Biochemistry - Vol. I* by Donald and Judith G. Voet and *Introduction to Macromolecular Crystallography* by Alexander McPherson.

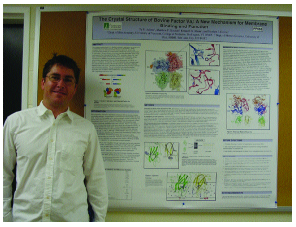
Conference of the Asian Crystallographic Association (AsCA; June 27-30; Hong Kong, China). The prize was awarded to Chin-Yu Chen for "Probing the DNA Kink Structure Induced by the Hyperthermophilic Chromosomal Protein SAC7D Using Site-Directed Mutagenesis and X-Ray Crystallography"



Chin-Yu Chen,[a-c] Ting-Wan Lin,[a] Chia-Cheng Chou,[a,b] Tzu-Ping Ko,[a] and Andrew H.-J. Wang[a,d]

[a]*Institute of Biological Chemistry and* [b]*Core Facility X-ray Crystallography, Academia Sinica, Taipei 115, Taiwan;* [c]*Department of Chemistry and* [d]*Institute of Biochemical Sciences, National Taiwan University, Taipei 106, Taiwan.*

The AsCA Judging Committee as organized by Peter Colman - TP Singh and Se Won Suh.

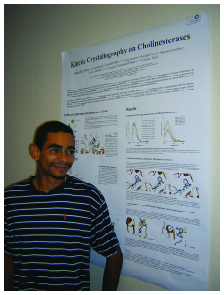


American Crystallographic Association's Annual Meeting (ACA; July 17-22; Chicago, IL). The prize was awarded to Ty Adams for "The Crystal Structure of Factor Va: A New Mechanism for Membrane Binding and Function"

T.E. Adams,[a] M.F. Hockin,[b] K.G. Mann,[a] S.J. Everse[a]

[a]*College of Medicine, University of Vermont, Burlington, VT 05401;* [b]*Howard Hughes Medical Institute, University of Utah, Salt Lake City, UT 84112.*

ACA Judging Committee as organized by Edward J. Collins - Jung-Ja Kim (Chair), Richard Brennan, Carolyn Brock, John Chrzas, and Nick Sauter.



22nd European Crystallographic Meeting (ECM 22; August 26-31; Budapest, Hungary). The prize was awarded to Jacques-Ph. Colletier for the poster "Kinetic crystallography on the cholinesterases"

J.P. Colletier,[a] A. Royant,[b] A. Specht,[c] F. Nachon,[d] G. Zaccai,[a] M. Goeldner,[c] J.L Sussman,[e] I. Silman,[f] D. Bourgeois,[b] and M. Weik[a]

[a]*LBM &* [b]*LCCP, IBS, Grenoble, France;* [c]*LCB, ULP, Strasbourg, France;* [d]*UE, CRSSA, La Tronche, France;* [e]*DSB &* [f]*DNB, WIS, Rehovot, Israel).*

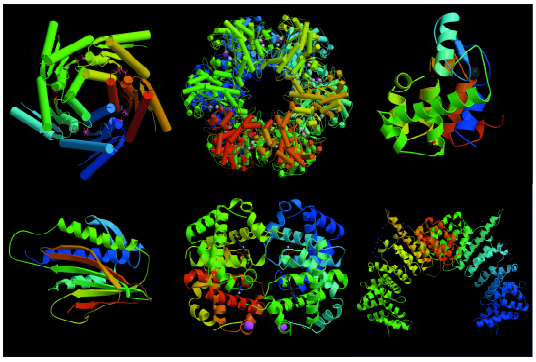
ECM 22 Judging Committee - Matthias Bochtler, Zsolt Bocskei, Stefania Di Marco, Andrea Hadfield, and the Chair, Vilmos Fulop.

The RCSB PDB Poster Prize contest will resume in 2005 - further details will be announced in RCSB PDB website news.

Art of Science at EMBL-Hamburg

EMBL-Hamburg hosted the conference "Structural Biology at Crossroads: From Biological Molecules to Biological Systems" on September 15-18. An exhibition of the RCSB PDB's Art of Science gallery show was opened during the second evening of the meeting with a presentation by RCSB PDB Director Helen M. Berman. Some of the best movies from the protein structure world were also shown.

The exhibit was on display in the DESY Bistro (Notkestr. 85, Hamburg, Germany) until October 03, 2004.



Images from the Art of Science *Exhibit*

"The Impact of Structural Genomics on the Protein Data Bank" Published

A paper describing structural genomics' effects on the PDB's data pipeline, data capture, and target tracking has been published in the *American Journal of PharmacoGenomics*:

The Impact of Structural Genomics on the Protein Data Bank

Helen M. Berman and John Westbrook

Am. J. Pharmacogenomics 2004; 4:247-252

New Data CD Released

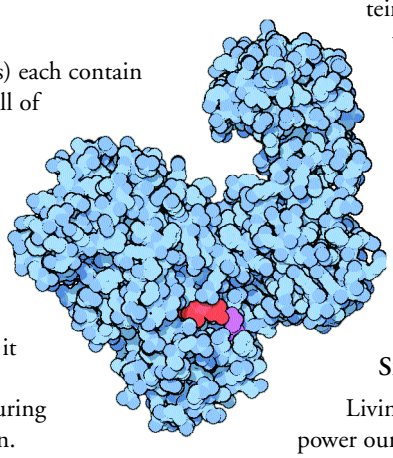
Two products were distributed for the July 2004 data CD release. Release 109U contains the incremental set of experimentally determined structures and models released between April 1, 2004 and July 1, 2004, and release 108U-EXP contains the experimental data (X-ray structure factors and NMR constraints) released during the same quarter. Each is on a single CD-ROM. Questions should be directed to **pdbcd@rcsb.org**. Ordering information is available at **www.rcsb.org/pdb/cdrom.html**.

PDB Molecules of the Quarter: DNA Ligase, Capases, & Catalase

The *Molecule of the Month* series by David S. Goodsell regularly explores the functions and significance of selected biological macromolecules for a general audience (www.rcsb.org/pdb/molecules/molecule_list.html). Structures highlighted during this past quarter were:

July 2004—*DNA Ligase*

Human cells (with a few unusual exceptions) each contain their own set of 46 long strands of DNA. All of our genetic information is encoded in these strands, with thousands of genes strung along their length. The ordering of genes, and the proximity of one next to the other, can be important for the proper usage of the information, so it is important that our cells protect their DNA from breakage. If one strand in the DNA breaks, it is not a disaster, but it can lead to problems when the DNA double helix is unwound during the processes of transcription and replication. Breakage of both strands, on the other hand, is far more serious. To protect us from these dangers, our cells use DNA ligases to glue together DNA strands that have been broken.



DNA Ligase. PDB ID: 1dgs

Lee, J.Y. Chang, C. Song, H.K. Moon, J. Yang, J.K. Kim, H.K. Kwon, S.T. Suh, S.W. Crystal structure of NAD(+)-dependent DNA ligase: modular architecture and functional implications. (2000) EMBO J. *19, 1119 -1129.*

DNA ligase reconnects DNA strands when they are broken. It uses a cofactor molecule for power and a special lysine amino acid to perform the reaction. Our DNA ligases and the DNA ligase from the bacteriophage T7 use ATP as the cofactor. Many bacteria, on the other hand, use NAD in the reaction. In both cases, a lysine in the DNA ligase forms a bond to the phosphate in the cofactor, holding onto the AMP portion and discarding the rest. Later in the reaction, this AMP is transferred to the broken DNA strand, and then is released when the strand is rejoined.

For more information on DNA ligase, see www.rcsb.org/pdb/molecules/pdb55_1.html.

August 2004—*Caspases*

Billions of cells in your body will die in the next hour. This is entirely normal – the human body continually renews itself, removing obsolete or damaged cells and replacing them with healthy new ones. However, your body must do this carefully. If cells are damaged, like when you cut yourself, they may swell and burst, contaminating the surrounding area. The body responds harshly to this type of cell death, inflaming the area by rushing in blood cells to clean up the mess. To avoid this messy problem, your cells are boobytrapped with a method to die cleanly and quickly on demand. When given the signal, the cell will disassemble its own internal structure and fragment itself into small, tidy pieces that are readily consumed by neighboring cells. This process of controlled, antiseptic death is called apoptosis.

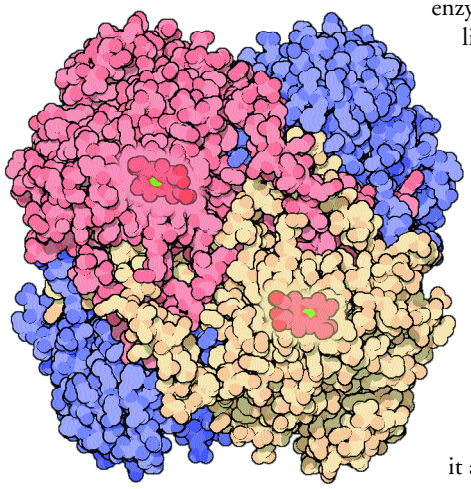
Caspases are the executioners of apoptosis. They are protein-cutting enzymes that chop up strategic proteins in the cell. The name refers to two properties of these enzymes. First, they are cysteine proteases that use the sulfur atom in cysteine to perform the cleavage reaction. Second, they cut proteins next to aspartate amino acids in their chains. They do not cut indiscriminately--instead, they are designed to make exactly the right cuts needed to disassemble the cell in an orderly manner.

For more information on caspases, see www.rcsb.org/pdb/molecules/pdb56_1.html.

September 2004—*Catalase*

Living with oxygen is dangerous. We rely on oxygen to power our cells, but oxygen is a reactive molecule that can cause serious problems if not carefully controlled. One of the dangers of oxygen is that it is easily converted into other reactive compounds. Inside our cells, electrons are continually shuttled from site to site by carrier molecules, such as carriers derived from riboflavin and niacin. If oxygen runs into one of these carrier molecules, the electron may be accidentally transferred to it. This converts oxygen into dangerous compounds such as superoxide radicals and hydrogen peroxide, which can attack the delicate sulfur atoms and metal ions in proteins. To make things even worse, free iron ions in the cell occasionally convert hydrogen peroxide into hydroxyl radicals. These deadly molecules attack and mutate DNA. One theory, still controversial, is that this type of oxidative damage accumulates over the years of our life, causing us to age.

Fortunately, cells make a variety of antioxidant enzymes to fight the dangerous side-effects of life with oxygen. Two important players are superoxide dismutase, which converts superoxide radicals into hydrogen peroxide, and catalase, which converts hydrogen peroxide into water and oxygen gas. The importance of these enzymes is demonstrated by their prevalence, ranging from about 0.1% of the protein in an *Escherichia coli* cell to upwards of a quarter of the protein in susceptible cell types. These many catalase molecules patrol the cell, counteracting the steady production of hydrogen peroxide and keeping it at a safe level.



Catalase. PDB ID: 8cat

Fita, I. Rossmann, M.G. The NADPH binding site on beef liver catalase. (1985) Proc.Natl.Acad.Sci.USA, 82, 1604-1608.

For more information on catalases, see www.rcsb.org/pdb/molecules/pdb57_1.html.

PDB Community Focus: Haruki Nakamura, PDBj

Haruki Nakamura is the Director of the Protein Data Bank Japan (PDBj) in Osaka, Japan, and one of the founding members of the wwPDB. Born in Tokyo, Japan, he received his Doctor of Science degree in physics at the Faculty of Science, University of Tokyo. His doctoral research resulted in a thesis titled 'Dielectric studies of the biological polyelectrolytes by Fourier-synthesized-pseudorandom-noise-dielectric spectrometer.' He began his post-graduate career as a Research Associate at the Department of Applied Physics Faculty of Engineering at the University of Tokyo. As a Visiting Researcher at the Astbury Department of Biophysics at Leeds University, Haruki studied molecular graphics in the laboratory of Professor A. C. T. North. He has also been a guest professor at a number of prestigious universities. In 1987, he became the Director of Second Department, Protein Engineering Research Institute (PERI) at Osaka, studying molecular modeling, design and analysis, and in 1996, he was named Research Director, Department of Bioinformatics, Biomolecular Engineering Research Institute (BERI) - a successive institute of PERI. In addition to being the director of PDBj, Haruki is currently a Professor in the Laboratory of Protein Informatics, at the Research Center for Structural and Functional Proteomics, Institute for Protein Research, Osaka University. Throughout his career his research interests have included biophysical studies of protein architecture, electrostatic properties and enzymatic functions, protein modeling, protein design, computational chemistry, and structural bioinformatics.

Q How did you come to be involved with the PDBj, and how has your own research influenced your vision for the PDBj?

A The Institute of Protein Research (IPR) at Osaka University has collaborated with the PDB since its foundation in the 1970s. However, up until five years ago, the collaboration had been very limited due to little governmental support. What I first did after moving to IPR was to emphasize the importance of the life science databases and bioinformatics technology, and to persuade the university and the government that IPR should contribute to the PDB database much more than before. Fortunately, my proposal to develop these areas -- to curate, edit, and distribute structural data, develop a new XML format with an XML-based browser, develop several secondary databases, and start a mirror site of BMRB -- was approved by our Japanese government, to accompany the structural genomics project in Japan. In order to promote all these activities, we founded a new organization called PDBj. The PDBj activity is not pure research, but provides many services to scientists, students, and general citizens all over the world; in particular, we have some responsibility for the Asian and Oceania regions. However, as a service provider, our knowledge areas now cover a much wider field: Crystallography, NMR, Informatics, Graphics, Web technology, and so on. In particular, our experience developing the canonical PDBML in collaboration with the RCSB PDB has increased our skills in XML and GRID computing. Development of our secondary databases provided a good opportunity to learn about integrating computational chemistry and information science.

Q What are your long-term goals for PDBj, especially in light of the rapid changes taking place in structural biology?

A With more protein and DNA structures being determined rapidly, every data curation and editing procedure should be automated as much as possible without sacrificing data quality. The raw experimental data should also be stored and distributed from the PDB. Thus, one of our long-term goals for the future is to establish a stable data management system as a sustainable system that will not require much manual effort or large financial support. This may be realized with the rapid development of data grid technology, in which the distributed data yielded by structural biologists may be gathered and integrated based on the grid architecture through the Internet. Otherwise, database services may not be sustainable in society. The introduction of XML for description and validation of PDB data is the very first step to this goal.

Q What is the nature of your interactions with the RCSB PDB and with EBI-MSD and what effect, if any, does the formation of the wwPDB have on these interactions?

A When we started PDBj, the collaborations with RCSB PDB and with EBI-MSD were essential, because PDBj is the newest entry in this field. Therefore, the PDBj members have frequently visited both RCSB PDB and EBI-MSD, and we have also invited people from RCSB PDB and EBI-MSD, for example, when we organized international workshops at IPR, Osaka University. The foundation of wwPDB should make these collaborations much tighter than before. I am looking forward to attending the first annual meeting of wwPDB this year.

Q Do you think that the wwPDB will be effective in providing for the long-term stability of the PDB archives?

A Sure. Structural genomics projects and most structural biology research rely upon financial support from the governments of individual countries. The data management should thus be made by several different countries collaborating with each other. Foundation of the wwPDB is one of the essential points to make PDB a sustainable international database.

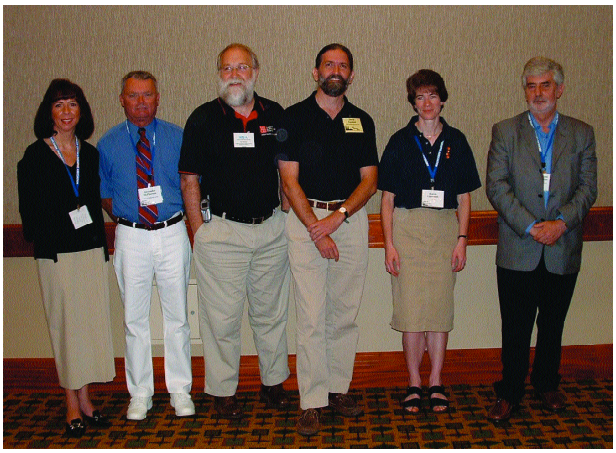
Q The amount of biological structure data is increasing almost exponentially. From your experience, what do you see as the overall future for databases that have to deal with this explosion of data?

A As mentioned previously, a stable data management system in the future should not require much manual effort or very huge financial support to be a sustainable system. Introducing a new procedure is inevitable, in which every data curation and editing procedure can be automated without losing any data quality. Development of PDBML for description and validation of PDB data is the very first step to this goal. In the near future, the processes and workflows required should be described using the standard ML technology. For that goal, more collaboration with computer scientists is necessary.

PDB Education Corner: *X-Rays, Molecules, and You* Workshop

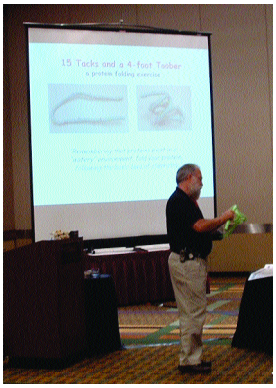
*This workshop was organized by the RCSB Protein Data Bank and co-sponsored by the ACA (*www.hwi.buffalo.edu/ACA*). This review is written by Shuchismita Dutta (RCSB PDB).*

It seems difficult to imagine bright-eyed high-school students and their proud teachers discussing structural biology on a summer Sunday morning. Yet this was the scene at the "X-rays, Crystals, Molecules and You" workshop held on July 18th 2004 at the Hyatt Regency Chicago during the American Crystallographic Association's annual meeting. During this workshop, prominent crystallographers and structural biologists introduced high school students and teachers to basic concepts in X-ray crystallography and structural databases to promote interest in structural biology, chemistry, and general science. This workshop generated enough interest that approximately 60 students, teachers, and parents traveled from 18 different states to participate. Several ACA members also attended the lectures. The morning session introduced crystallography concepts, highlighted structural databases, and discussed representational models of structures as teaching tools. Two mini-workshops followed in the afternoon - crystallization for teachers, and modeling and visualization of structures for students.



Speakers, from left to right: Katherine Kantardjieff, Alexander, Alexander McPherson, Tim Herman, David S. Goodsell, Karen Lipscomb, and Frank Allen. Tommie Hata is not pictured.

Judith L. Flippen-Anderson, the production and outreach leader at the RCSB PDB, began the morning session with a brief welcome address. Katherine Kantardjieff, professor of physical chemistry at California State University Fullerton and director of the W.M. Keck Center for Molecular Structure, followed by introducing the concepts and procedures involved in the practice of X-ray crystallography. She described how crystals of proteins and other molecules are grown, harvested, and used for data collection. Kantardjieff then discussed how the data collected relate to electron density maps and how these these maps are used to build a model of the structure and generate 3-dimensional coordinates for each atom. Kantardjieff shared her somewhat circuitous route to becoming a crystallographer, and encouraged students and teachers to continue working towards their goals.



Tim Henman demonstrates hands-on protein folding

The second lecture discussed the data, tools and resources available at the Cambridge Crystallographic Data Center (CCDC; www.ccdc.cam.ac.uk). Frank Allen, the executive director of CCDC, explained how crystallography is used to determine the structures of molecules ranging from small metal ions to very large viruses. In all cases, this method provides an understanding of the shape, size, dimensions and interactions of the molecule being studied. He then focused on the structures present in the Cambridge Structural Database (CSD), the world repository of the small molecule crystal structures and the principle product of the CCDC. Allen described the different classes of molecules in the CSD and the ways in which the CSD can be used, including predicting where some of these small molecules may bind in an enzyme active site or binding pocket. Scientific Support Manager Karen Lipscomb then demonstrated some of the tools and resources available at the CCDC by querying the database for the Nobel Prize-winning structures solved by Dorothy Hodgkin and creating structure images.

Then David Goodsell, associate professor in the Department of Molecular Biology at the Scripps Research Institute, discussed how the structural data present in the PDB archives are used for research and education. The growing PDB archive contains the three-dimensional coordinates and related information about biological macromolecules. These structures, including proteins, nucleic acids, and large macromolecular complexes, provide insight into these molecules' roles in fundamental biological processes. Goodsell is also the illustrator and primary author of the RCSB PDB's Molecule of Month educational feature. He presented a historic overview of how the atoms that make up proteins, nucleic acids and other molecules in the PDB have been visually represented by hand drawings, wire-frame, backbones, space-filling models and finally as ribbons. He demonstrated how each representation highlights different aspects and features of molecules.

The final lecture in the morning session was jointly presented by Tim Herman, Director of the Center for BioMolecular Modeling

(CBM) at the Milwaukee School of Engineering, and Tommie Hata, a high school teacher at the Pingry School in Martinsville, NJ. Tim Herman started off by describing how physical models act as "thinking tools" and can make molecular structures "real" for researchers, teachers, and students alike. He briefly described how he uses the 3-D coordinates from the PDB archives to generate physical models of proteins. He also distributed a kit containing a pliable 4-foot tube and colored thumbtacks designed to demonstrate concepts in protein folding and interaction (see www.3dmoleculardesigns.com). The student-teacher workshops organized by his center to promote an understanding of molecular structure through physical models were discussed. Tommie Hata had attended one of these workshops, following which he involved some of his own students in CBM's "Students Modeling A Research Topic" (SMART) team program. Hata talked about his SMART team's experiences, which included working with research scientists to create a physical model of a class I transcription activation complex.

David S. Goodsell and a SMART team at the poster session at the ACA meeting

Following lunch, teachers and students participated in different activities. Alexander McPherson, professor of molecular biology and biochemistry at University of California at Irvine, led the teachers through a hands-on exercise in crystallizing lysozyme. McPherson was awarded the ACA's prestigious Fankuchen Award later in the meeting for his many significant contributions, including his work in crystallization, and determination of various plant viruses, immunoglobulins and other molecules. Meanwhile, Goodsell, Herman, and Lipscomb led the students in various exercises. They explored the RCSB PDB, and located, downloaded and viewed a structure of a DNA-binding protein containing zinc finger domains. The students were challenged to search for and visualize estrogen and testosterone in the CSD in a short time period. They then used the tube kit to model a single zinc finger domain based on what they downloaded and examined from the PDB. The students also explored the exhibitor booths and poster presentations at the ACA meeting. Several students presented posters at the ACA meeting about their own SMART projects.

The workshop provided a great opportunity for students and teachers to learn about crystallography and structural biology alongside expert research scientists in their field.

Related Links: Database Challenges in Biology Symposium

These links are related to the presentations given at the RCSB's "Databases Challenges in Biology" symposium held on September 10 at CARB.

Biomedical Informatics Research Network (BIRN; nbirn.net)

Multi-scale Imaging and Databasing of the Nervous System with Advanced Cyberinfrastructure, *Mark Ellisman, University of California, San Diego*

National Center for Macromolecular Imaging (ncmi.bcm.tmc.edu/ncmi)

Database for Cryo-Electron Microscopy, *Wah Chiu, Baylor College of Medicine*


Speakers, from left to right: John E. Johnson, Wah Chiu, Mark H. Ellisman, Helen M. Berman, John L. Markley, Stephen H. Bryant, Cathy H. Wu

VIrus Particle ExploreR (VIPER; mmtsb.scripps.edu/viper)

VIrus Particle ExploreR (VIPER): a Database of Standardized Atom Coordinates for Icosahedral Viruses and Derived Descriptions of Subunit Interactions, *John Johnson, The Scripps Research Institute*

Center for Eukaryotic Structural Genomics (CESG; uwstructuralgenomics.org) and BioMagResBank (BMRB; www.bmrb.wisc.edu)

Data Management in the Laboratory: User Facilities and Research on Small and Large Scales, *John Markley, University of Wisconsin-Madison*

CDD: A Conserved Domain Database (www.ncbi.nlm.nih.gov/Structure/cdd/cdd.shtml)

Conserved Domain Database: A Protein Family Database, *Stephen Bryant, National Center for Biotechnology Information*

Protein Information Resource (pir.georgetown.edu)

PIR Integrated Bioinformatics for Functional Genomics and Proteomics, *Cathy Wu, Georgetown University Medical Center*

RCSB PDB (www.pdb.org) and RCSB PDB Beta (pdbbeta.rcsb.org)

The RCSB Protein Data Bank: An Integrated Resource for Structural Biology, *Helen M. Berman, Rutgers, The State University of New Jersey*

RCSB PDB Partners

The RCSB PDB is managed by three partner sites of the Research Collaboratory for Structural Bioinformatics:

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