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RCSB PDB PROTEIN DATA BANK NEWSLETTER

Weekly RCSB PDB news is available online at www.pdb.org

Contents

SNAPSHOT: JANUARY 1, 2009

55072 released atomic coordinate entries

50854	proteins, peptides, and viruses
1949	nucleic acids
2236	protein/nucleic acid complexes
33	other

EXPERIMENTAL TECHNIQUE

47132	X-ray
7627	NMR
209	electron microscopy
104	other

36256 structure factor files
4313 NMR restraint files

Participating RCSB Members:
Rutgers • SDSC/SKAGGS/UCSD
E-mail: info@rcsb.org
Web: www.pdb.org • FTP: ftp.wwpdb.org

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

Message from the RCSB PDB

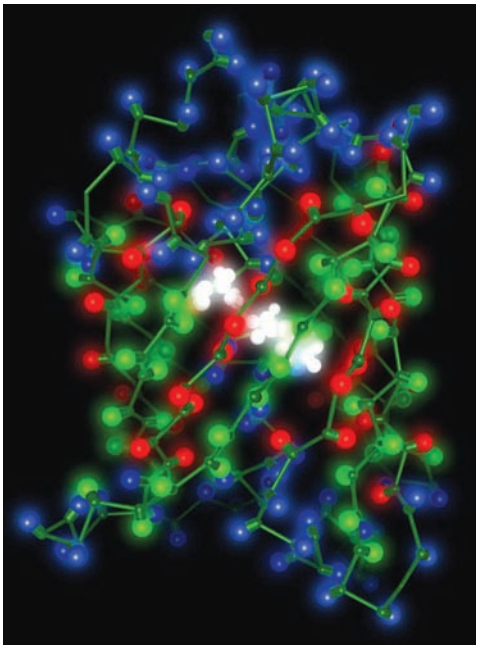
In 2008, the RCSB PDB reached several milestones and released many new resources.

The 50,000th structure was released in the PDB archive in April, and by the end of December, more than 55,000 structures were available. All of these structures offer opportunities for learning–whether through their novelty, complexity, or even their similarity with other structures.

April's *Molecule of the Month* feature on adrenergic receptors was the 100th installment of the series. Since January 2000, *Molecule of the Month* has explored the structure and function of proteins and nucleic acids found in the PDB archive such as transfer RNA, anthrax toxin, and multidrug resistance transporters. By highlighting these structures, this ongoing feature provides a good entry point for navigating through all of the structures available in the PDB archive.

Another educational resource, the recently-released *Looking at Structures*, is intended to help researchers and educators get the most out of the PDB archive. Broad topics include how to understand PDB data, how to visualize structures, how to read coordinate files, and potential challenges to exploring the archive.

For depositors, a variety of tools were released to help streamline the deposition process. Resources such as **SF-Tool**, which validates and translates structure factor files, and **Ligand Expo**, which can be used to search and build chemical components, join proven resources such as **pdb_extract** and **ADIT**. The wwPDB's publication of the Comprehensive Format Guide Version 3.2 marks another achievement towards the standardization of the archive.



Website features, including the enhanced RSS feed, 3D views of domain information, and *Advanced Search*, offer a diverse tool set for accessing PDB data.

These features were all developed with input and feedback from our diverse user community. We look forward to this continued collaboration in 2009.

*This image of green fluorescent protein was created by David S. Goodsell using the Python Molecular Viewer (**mgltoools.scripps.edu**). Structure shown is PDB ID 1gfl (F. Yang, L.G. Moss, G.N. Phillips Jr. (1996) The molecular structure of green fluorescent protein.* Nat.Biotechnol. *14: 1246-1251).*

Data Deposition and Processing

PDB Archive Version 3.15 to be Released

A new standardized version of the PDB archive will be available from ftp://ftp.wwpdb.org in early 2009. The date will be announced at wwpdb.org.

As of December 2, 2008, all new PDB releases follow PDB File Format Contents Guide Version 3.20. With the new version of the archive, all entries released prior to December 2, 2008 will be re-released as PDB Format Version 3.15 files. This release will overwrite all existing files.

A snapshot of the archive before this release will be available from ftp://snapshots.wwpdb.org/.

Tools for downloading the archive can be found at www.wwpdb.org/downloads.html.

For file format documentation, please see www.wwpdb.org/docs.html.

Questions may be sent to info@wwpdb.org.

Tips for Depositing Multiple Related Structures using ADIT/ADIT-NMR

For depositing many structures that are related to one another, there are a few ways of making the ADIT/ADIT-NMR deposition process simpler:

- Use pdb_extract when preparing structures solved using X-ray crystallography or NMR. Not only does pdb_extract minimize the amount of manual typing needed during the deposition process, it also utilizes an author information form that can be filled out just one time for use with multiple entries.

pdb_extract takes information about data collection, phasing, density modification, and the final structure refinement from the output files and log files produced by the various applications used for structure determination. The collected information is organized into a file ready for deposition using ADIT/ADIT-NMR.

The *author information form* in pdb_extract contains author names, citation information, protein names and source--the types of information that are repeated in multiple related entries. This form can be filled out once and used with pdb_extract to prepare several structures for deposition.

- For structures solved by other experimental methods, first deposit one representative structure. After it has been annotated and processed, use this finalized entry as a template for the related depositions by replacing the coordinates and updating information in the PDB or mmCIF file as necessary.

- If the structures have bound ligands, drugs, or inhibitors, please check Ligand Expo for matching chemical components. If a match is found, use that corresponding ID code for the component in your coordinates. If a match is not found, choose a new three-character code for the component, and upload the chemical name and a file showing the chemical drawing for the new component into the Ligand Information section of ADIT/ADIT-NMR.

These resources and more can be found at www.pdb.org.

2008 Deposition Statistics

In 2008, 7043 experimentally-determined structures were deposited to the PDB archive.

The entries were processed by wwPDB teams at the RCSB PDB, PDBe, and PDBj. Of the structures deposited in 2008, 75.7% were deposited with a release status of "hold until publication"; 19.5% were released as soon as annotation of the entry was complete; and 4.8% were held until a particular date.

90.9 % of these entries were determined by X-ray crystallographic methods; 8.1% were determined by NMR methods. Since February 1, 2008, depositing structure factor amplitudes/intensities (for crystal structures) and restraints (for NMR structures) has been a mandatory requirement for PDB deposition. As a result, 98.7 % of the 2008 depositions were deposited with experimental data.

Also in 2008, 7072 structures were released into the archive.

Data Query, Reporting, and Access

2008 Website Statistics

2008 access statistics for www.pdb.org are given below. Download statistics are available from www.wwpdb.org.

Month	Unique Visitors	Number of Visits	Bandwidth
JANUARY	128781	319459	426.87 GB
FEBRUARY	139444	338946	567.18 GB
MARCH	152264	361999	642.98 GB
APRIL	134119	309222	585.77 GB
MAY	123862	286612	607.73 GB
JUNE	132168	317814	651.02 GB
JULY	161567	355065	636.25 GB
AUGUST	133412	296024	514.27 GB
SEPTEMBER	168114	366983	631.13 GB
OCTOBER	178581	404453	843.63 GB
NOVEMBER	173891	381565	728.30 GB
DECEMBER	141294	303359	491.65 GB

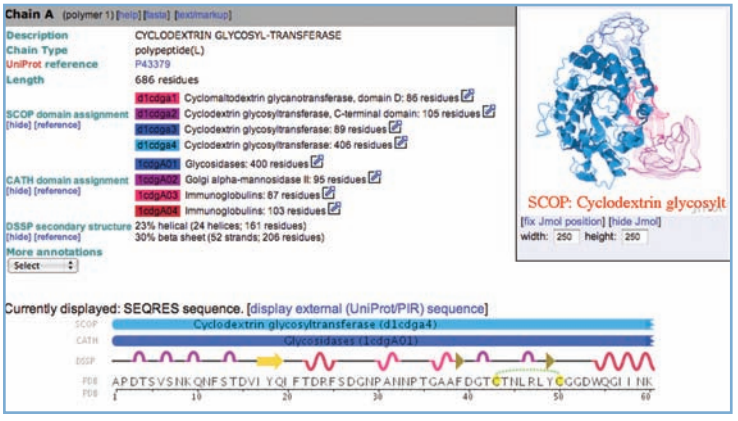
View Domain Annotations in 3D

Sequence Details pages for all protein structures now include a Jmol view of the structure that can display domain annotations from SCOP, CATH, DP, PDP, Pfam, and InterPro.

To activate this view from a structure summary page, first select the Sequence Details tab. The default view displays a 2D graphical representation of the UniProt, PDB-ATOM and PDB-SEQRES sequences. Users can also select third-party domain annotations from this 2D image to appear with the corresponding structure in a Jmol viewer.

To view these annotations mapped onto the 3D structure, select [**show 3D in Jmol**] from the top of the page. Then, click on any of the domains on the sequence view. The corresponding colors for that domain will appear in the 3D Jmol viewer. The annotations shown in Jmol can change by clicking on an annotation shown in the 2D view.

By default, the Jmol window stays positioned on the top of the page. Select [**dynamic Jmol position**] to have the Jmol viewer adjust so that it is always to the top right of the page as you scroll down.



2D and 3D representations of sequence and domain annotations for PDB entry 1cdg (C.L. Lawson, R. van Montfort, B. Strokopytov, H.J. Rozeboom, K.H. Kalk, G.E. de Vries, D. Penninga, L. Dijkhuizen, B.W. Dijkstra (1994) Nucleotide sequence and X-ray structure of cyclodextrin glycosyltransferase from Bacillus circulans *strain 251 in a maltose-dependent crystal form.* J.Mol.Biol. *236: 590-600).*

References:

Jmol: www.jmol.org
SCOP: scop.mrc-lmb.cam.ac.uk/scop
CATH: www.cathdb.info
DP: compbio.ornl.gov/structure/domainparser
PDP: 123d.ncifcrf.gov/pdp.html
Pfam: pfam.sanger.ac.uk
InterPro: www.ebi.ac.uk/interpro

Getting Started with the RCSB PDB Website

Not sure how to find what you're looking for? To help users access all of the data and related resources available from the RCSB PDB website, the *Getting Started* page has been updated. This introduction offers a quick start to using the website and explains the left-hand menu and the tabbed navigation system. For example, selecting each tab offers rich ways of exploring individual structures and search result sets. The left-hand menus organize resources by topic.

The *Getting Started* page is available from the bottom of www.pdb.org.

Browser Check for Compatibility with Website Features

Is your web browser configured to fully utilize RCSB PDB website features such as changing menus, temporarily stored queries, and Advanced Search? Click on the browser check page from the bottom of www.pdb.org to find out.

Most modern browsers are fully supported. Users may encounter difficulty in certain portions of the site when using unsupported browsers or when different options are turned off.

The browser check page reports if there are any problems with your browser or browser settings, and provides instructions if changes are needed. Any other questions or problems? Please let our help desk know at info@rcsb.org.

Browser Information: Mozilla Firefox 2.0.0.17

Description	Status	Details	Notes
JavaScript	✓ Pass	JavaScript is enabled in your browser.	
Cookies	✗ Fail	Cookies are disabled in your browser.	*To enable cookies in your browser, follow the instructions below* 1. Select 'Options...' from the 'Tools' menu. 2. Click on the 'Privacy' tab at the top of the window. 3. In the 'Cookies' section, set 'Accept cookies from sites' check box. 4. Click the 'OK' button to close the Options window.
Java	✓ Pass	Java version 1.5.0_16	
Popup windows	✓ Pass	Popup windows are enabled in your browser.	

The browser check report

Outreach and Education

Meetings and Presentations

The RCSB PDB has been participating in a wide variety of meetings:

• At the New Jersey Science Convention (NJSC; October 14-15; Somerset, NJ), science teachers visiting the RCSB PDB booth learned about the structures in the PDB archive and the RCSB PDB materials available for use in their classrooms. Many teachers also created virus structures during a presentation by Shuchismita Dutta.

• John Westbrook described the Chemical Component Dictionary and Ligand Expo at the eCheminfo *Community of Practice Meeting on Advances in Drug Discovery and Development* (October 13-17; Philadelphia, PA).

• During the meeting of the Association of Science and Technology Centers (ASTC; October 18-21; Philadelphia, PA), science museums representatives and content developers met David Goodsell and Christine Zardecki at the exhibit booth to learn about the resources available for visualizing structures available from the RCSB PDB.

• Huanwang Yang presented a poster about online tools such as pdb_extract and SF-Tools at the Pittsburgh Diffraction Conference (October 30-November 1; Pittsburgh, PA).

• At the Cold Spring Harbor Course *X-Ray Methods In Structural Biology* (October 13-28), John Westbrook presented "PDB Tools in Deposition".

Many teachers created virus structures with the RCSB PDB at the New Jersey Science Convention.

At the Association of Science and Technology Centers meeting, science museum content developers picked up resources and materials at the RCSB PDB exhibit booth.

• Shuchismita Dutta described the evolving PDB resource and the wwPDB in a poster at the EMBO World Lecture Course *Recent Developments in Macromolecular Crystallography* (November 9-14, 2008; Pune, India).

Future meetings include the Keystone Symposia *Frontiers of NMR in Biology* (February 15 - 20, 2009; Santa Fe, NM) and the Biophysical Society Annual Meeting (February 28 - March 4, 2009; Boston, MA). The RCSB PDB will also be participating in the San Diego Science Festival and Rutgers Day this spring. Details will be announced at www.pdb.org.

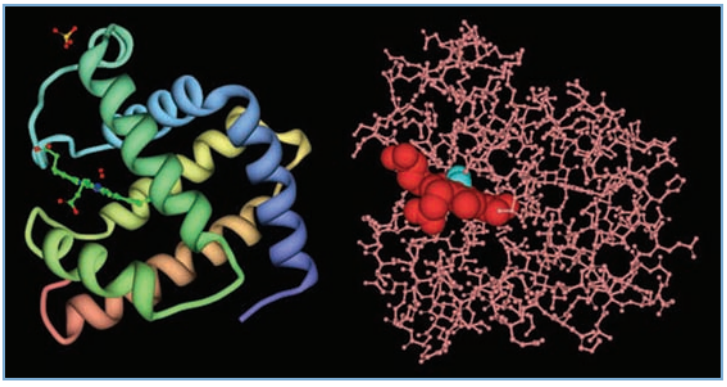
Looking at Structures: A Resource for Learning About PDB Data

Where are all the hydrogen atoms in this file? Should I care about the R-factor? Why are there 20 overlapped structures in my file? These questions and many others are explored in the RCSB PDB's new *Looking at Structures* online resource.

Using text, images, and interactive Jmols, *Looking at Structures* intends to help researchers and educators get the most out of the PDB archive. Broad topics include how to understand PDB data, how to visualize structures, how to read coordinate files, and potential challenges in exploring the archive.

A **Table of Contents** appears on the right side of every page so at any time, users can access the individual pages: **Biological Units**, **Dealing with Coordinates**, **Methods for Determining Structure**, **Missing Coordinates and Biological Units**, **Molecular Graphics Programs**, **Resolution**, and **R-value and R-free**.

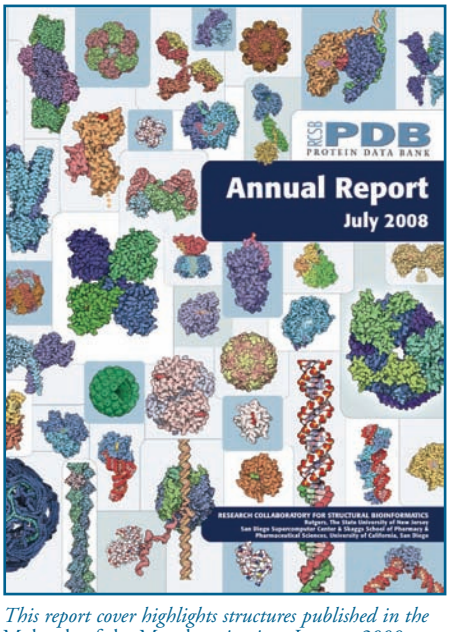
Looking at Structures is available from the General Education section of the left-hand menu at www.pdb.org.



From the Looking at Structures *chapter on Dealing with Coordinates. The left image shows myoglobin (PDB entry 1mbo) using the default representation in MBT Protein Workshop. It shows a ribbon diagram for the protein, and ball-and-stick for the small molecules. In the right image, we have changed the representation to show all atoms, using the information in each atom record to color the molecules differently. This clearly shows the heme group in bright red, and a bound oxygen molecule in turquoise.*

1mbo: S.E. Phillips (1980) Structure and refinement of oxymyoglobin at 1.6 Å resolution. J.Mol.Biol. *142: 531-554.*

Publications: 2008 Annual Report and More



This report cover highlights structures published in the Molecule of the Month *series since January 2000.*

The 2008 Annual Report features current progress and accomplishments, and explores the RCSB PDB's different activities in data deposition, query, and education.

The 2008 report highlights milestones, such as the publication of the 100th installment of the *Molecule of the Month*, and online resources such as Advanced Search. This publication is currently being distributed to the diverse community of PDB users in academia, industry, and education. If you would also like a printed copy, please send your postal address to info@rcsb.org.

Interested in an *Education Corner* from an older newsletter? Want to know what papers have been published that discuss the RCSB PDB project?

Looking for a flyer to guide you through the deposition process? The *News and Publications* page offers access to all RCSB PDB publications. Located in the General Information section of the left-hand menu, this page archives our Annual Reports on the history, mission, and yearly accomplishments of the project; publications in peer-reviewed journals; weekly news items about recent features and upcoming events; the quarterly newsletter; and more. Requests for printed copies may also be sent to info@rcsb.org.

To request printed versions of any RCSB PDB publications, please send your mailing address to ***info@rcsb.org****.*

RCSB PDB PROTEIN DATA BANK

THE RCSB PDB IS LOOKING FOR NEW PEOPLE TO JOIN OUR TEAM. POSITIONS INCLUDE:

CURRENTLY AVAILABLE JOB OPENINGS

- **JAVA DEVELOPER**
- **SCIENTIFIC SOFTWARE DEVELOPER**
- **SYSTEM ADMINISTRATOR**

FOR MORE DETAILS, PLEASE SEE THE RCSB PDB JOB LISTINGS PAGE AT WWW.PDB.ORG.

Education Corner by Bernadette Uzzi, Coordinator

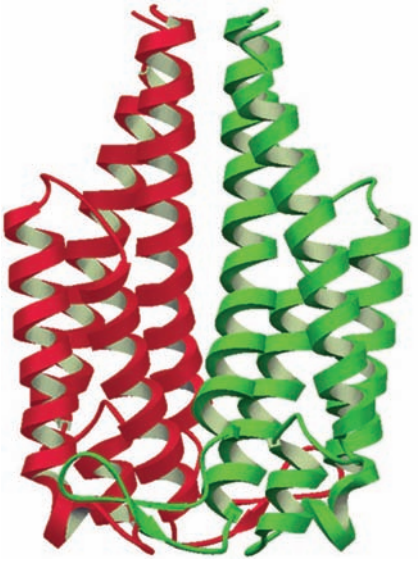
The Science Learning Center at Brookhaven National Laboratory

Many science educators face the challenge of successfully making the connection between what is learned in a classroom and "real" science. At Brookhaven National Laboratory's Science Learning Center, the two go hand in hand; its science-based educational facility is located within a world-class scientific research facility. The Science Learning Center offers hands-on lab experiences encompassing such disciplines as biology, chemistry, physics, and nanotechnology for secondary level students. These programs are aligned with the National Science Education Standards, and each program highlights the Laboratory's scientific research and achievements.

The Protein Data Bank (PDB) originated at Brookhaven in 1971 and was managed by the Lab until 1999. Many of the protein structures stored in the PDB were experimentally determined using intense X-ray beams at the Laboratory's National Synchrotron Light Source (NSLS). Many important discoveries were made at the NSLS. For example, the discovery of key proteins, OspA and OspC, located on the outer surface of the bacterium that causes Lyme disease, led to the development of Lyme vaccines for humans. Also at this laboratory, scientists were able to get a three-dimensional image of a virus enzyme, adenovirus protease, which may lead to the development of new anti-viral drugs. Both of these protein structures can be found in the PDB.

How does this complex information get translated to a level that a middle school student can understand? The answer: through hands-on science. At the Science Learning Center, we focus on making abstract scientific concepts real using activities grounded in research done at BNL. We offer a variety of classes on challenging subjects, including *DNA Extraction*, *Gene Transfer and Genetic Engineering*, and *Protein Structural Biology in 3D: The Shape of Things to Come*. These classes are scalable, so they can offer an introduction to the material for students or reinforce what was already learned in their classrooms as needed.

BERNADETTE UZZI (buzzi@bnl.gov) *is the Coordinator of Brookhaven National Laboratory's Science Learning Center. She holds a Bachelors degree in biology from the State University of New York at Potsdam, and has been teaching informal science for the past six years. Her additional responsibilities include developing and collaborating on educational programs specifically related to the Lab's research, and coordinating the Lab's Elementary School Science Fair and Middle School MagLev Contest.*



Researchers at NSLS determined the structure of OspC as seen in PDB IDs 1f1m and 1ggq (D. Kumaran, S. Eswaramoorthy, B.J. Luft, S. Koide, J.J. Dunn, C.L. Lawson, S. Swaminathan (2001) Crystal structure of outer surface protein C (OspC) from the lyme disease spirochete, Borrelia burgdorferi. EMBO J. *20: 971-978)*

Students come to the Science Learning Center to build cell models and perform DNA extractions. They genetically transform bacteria with a jellyfish gene, Green Fluorescent Protein (GFP), and culture the green bacteria that fluoresce under UV light. Students purify the GFP and learn how scientists use this same technique. The students don stereographic glasses and view a variety of molecules, including GFP, in a 3D visualization theater. Our educators make the connection between DNA, protein shape and function, and how that function is expressed as a trait. The students have the opportunity to use a tool that scientists at Brookhaven use, the PDB. The students are given laptop computers so they can search for the GFP structure. They manipulate the protein nicknamed the "light in the can" and seek out additional fluorescent proteins and make comparisons to the structures and traits. Students are encouraged to continue this research on their own.

Students viewing proteins

Using scientific tools is an effective way to motivate and excite students of all ages about science. Developing an understanding of why it is important and relevant to everyday life is a challenge. The Science Learning Center has found great success in bridging the gap between classroom learning and world-class scientific research.

Brookhaven National Laboratory's National Synchrotron Light Source

The Office of Educational Program's Science Learning Center (**www.bnl.gov/slc**) offers programs to students in grades 1-12, featuring interactive exhibits, hands-on labs, and programs that demonstrate basic scientific principles and utilize the inquiry method of teaching.

Brookhaven National Laboratory is operated and managed for the U.S. Department of Energy's Office of Science by Brookhaven Science Associates, a limited-liability company founded by the Research Foundation of the State University of New York on behalf of Stony Brook University and Battelle, a nonprofit, applied science and technology organization.

PDB Community Focus

Johannes Kirchmair, Ph.D., and Gerhard Wolber, Ph.D.
University of Innsbruck

Q: ***You recently published an extensive paper describing the PDB archive, its history, and related resources. What surprised you when you were preparing this manuscript?***

A: We were overwhelmed by the number and diversity of tools provided by the PDB portals and related websites. Before this work, we regularly used only a small part of PDB-related tools, simply because we were accustomed to them. After beginning to thoroughly investigate services and software available for structure-based PDB-related drug development, we immediately started using many of these tools and applications for research as well as for teaching. Another positively surprising fact was that many of

Drs. Kirchmair and Wolber are coauthors of the recently published *The Protein Data Bank (PDB), Its Related Services and Software Tools as Key Components for In Silico Guided Drug Discovery.*

Johannes Kirchmair, Patrick Markt, Simona Distinto, Daniela Schuster, Gudrun M. Spitzer, Klaus R. Liedl, Thierry Langer and Gerhard Wolber (2008) *J. Med. Chem.* 51: 7021–7040

pubs.acs.org/doi/abs/10.1021/jm8005977

these approaches take care of small organic ligands, while providing a high level of cross-linking; *i.e.*, it becomes possible to solve a specific problem by jumping from one service to another one without losing intermediate results. The best thing is that most of these services are free for non-commercial use despite their high quality. Naturally, this is great for teaching students, since we have access to a similar level of information as an industrial environment. The PDB bridges the two worlds of biology (macromolecules) and of medicinal chemistry (small molecules); it also provides a large quantity of easy-to-use tools for scientists that may not have been too much involved in computational chemistry or modeling so far. We see a strong trend for chemists to use PDB data to derive new ideas for synthesis and SAR within a short time without the need for installing any software; everything's on the web–free for academics!

Q: ***What do you think your online category of PDB-related tools (www.uibk.ac.at/pharmazie/phchem/camd/pdbtools.html) will look like in 10 years?***

A: Looking at the development in the past few years, we hope–and are confident–that ligand chemistry will become more important to the PDB. A tighter integration with initiatives like PubChem certainly bears great potential, such as being able to correlate ligand similarity with binding pocket similarity, which could lead to integrating virtual screening tools into the web interface of the PDB. 3D pharmacophores could be a good way to formulate the interaction of a ligand with its surrounding protein. Another possibility is that more software could be developed to further analyze the binding site. Protein-ligand-docking is also an interesting but currently controversial topic. If docking were to be regarded less commercially, eventually the PDB could offer a freely parameterizable docking toolbox that could help solving the scoring problem by large-scale statistics. We also hope that there will be more membrane proteins crystallized in the next 10 years, which would trigger the creation of a plethora of new tools that deal with membrane-drug interactions and homology modeling.

Q: ***How do you use the PDB when training pharmacy students?***

A: The RCSB PDB is an invaluable resource for teaching: the web application has improved so much in the past few years that many aspects of computational chemistry teaching can be directly covered using the standard RCSB PDB interface. Visualization of the proteins and binding pockets are only one; the ability to perform sequence similarity searches and the EC-classification to identify similar proteins with and without bound ligands are others. We also use the PDB as input to our own tools, such as the 3D pharmacophore generator LigandScout for developing structure-based 3D pharmacophores. For teaching medicinal chemistry, the clarity of the RCSB PDB web interface allows for demonstrating essential structure-activity relationships (*e.g.*, Which geometric chemical features are essential for ligand binding? If there is a reactive group on the ligand, why is an irreversible inhibitor bad? The PDB structure complex can show that the ligand is covalently bound to its co-factor).

Q: ***What are some challenges facing structure-based drug discovery today?***

A: The ligand affinity problem: protein-ligand docking has frequently addressed, but never solved this challenge. The practical approach that most scientists choose is to define rule-based scoring functions for their problems, and for that the PDB can help to better understand a problem by providing experimental data. However, there are still several issues with how the PDB stores small organic molecules. In some cases, it is still impossible to get the correct chemistry of a ligand from the PDB in an automated way. Sometimes, crystallographers do not pay much attention to the ligand or crystal waters and ions. Hence, it could be useful to store initial, un-refined electron densities without model bias only for the ligand to allow for re-interpretation. Other challenges are the lack of crystal structures for important protein classes, such as membrane proteins, and protein flexibility, especially conformational flexibility at the binding site which could be analyzed by multiple X-ray structures of one and the same target interaction site with multiple ligands.

Q: ***What are some of the new exciting opportunities in drug discovery? What role would the PDB play in these?***

A: The large collection of useful tools shows that the PDB provides extremely useful data for drug discovery–also for regarding small molecules, which probably has never been the primary focus of the PDB. Ligand Expo shows that ligands are becoming important, and we see a huge potential in paying more attention to ligand chemistry. Getting correct ligands directly from the PDB bears the potential of providing a lot of new cross-linking applications. Structure-based parallel screening and polypharmacology approaches are exciting topics that seem to be tailored for a database like the PDB.

JOHANNES KIRCHMAIR *studied pharmacy at the Leopold-Franzens University of Innsbruck, Austria, from 1999 to 2004 and received his Ph.D. degree under the guidance of Professor Thierry Langer in 2007. For his Ph.D., he specialized in structure-based virtual high-throughput screening and parallel screening techniques. His career began at Inte:Ligand GmbH in Vienna, Austria, working on computer-guided drug development using 3D virtual high-throughput screening techniques for the identification and optimization of novel anticancer agents. His research interests cover medicinal chemistry, computational chemistry, and drug design as well as QSAR and 3D-QSAR molecular modeling techniques. Since April 2008, Dr. Kirchmair has been a researcher at the University of Innsbruck and teaches computational chemistry.*

GERHARD WOLBER *received his Ph.D. in pharmaceutical chemistry at the University of Innsbruck in 2003 after his studies of computer science and pharmacy at the University of Innsbruck and University of Vienna, Austria, respectively. As one of the founders of the drug design company Inte:Ligand, he has been working as head of cheminformatics and research since 2003, where he has been developing the two programs ilib diverse and LigandScout. In 2008, he took a position as a lecturer in pharmaceutical chemistry at the Institute of Pharmacy at the University of Innsbruck, where he now heads his own research group and teaches computational and medicinal chemistry. His research interests include structure- and ligand-based drug design, efficient algorithms for virtual screening, 2D and 3D visualization techniques, and 3D pharmacophore modeling.*

Information about the Computer-aided Molecular Design group at the University of Innsbruck is available at **www.uibk.ac.at/pharmazie/phchem/camd.**

RCSB PDB Partners

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

Rutgers, The State University of New Jersey
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Chemical Biology
610 Taylor Road
Piscataway, NJ 08854-8087

San Diego Supercomputer Center and the Skaggs School of Pharmacy and Pharmaceutical Sciences
University of California, San Diego
9500 Gilman Drive
La Jolla, CA 92093-0537

The RCSB PDB is a member of the Worldwide Protein Data Bank (www.wwpdb.org)

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A list of current RCSB PDB Team Members is available from www.pdb.org.

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