Summer 2012 • Number 54

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Research Collaboratory for Structural Bioinformatics Protein Data Bank

# RCSB PDB PROTEIN DATA BANK NEWSLETTER

www.rcsb.org • info@rcsb.org

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

## Contents



## SNAPSHOT: JULY 1, 2012

82679 released atomic coordinate entries

**ENTRIES BY MOLECULE TYPE**

| | |
|---|---|
| 76537 | proteins, peptides, and viruses |
| 2388 | protein/nucleic acid complexes |
| 3731 | nucleic acids |
| 23 | other |

**ENTRIES BY EXPERIMENTAL TECHNIQUE**

| | |
|---|---|
| 72543 | X-ray |
| 9487 | NMR |
| 436 | electron microscopy |
| 50 | hybrid |
| 163 | other |

**RELATED EXPERIMENTAL DATA FILES**

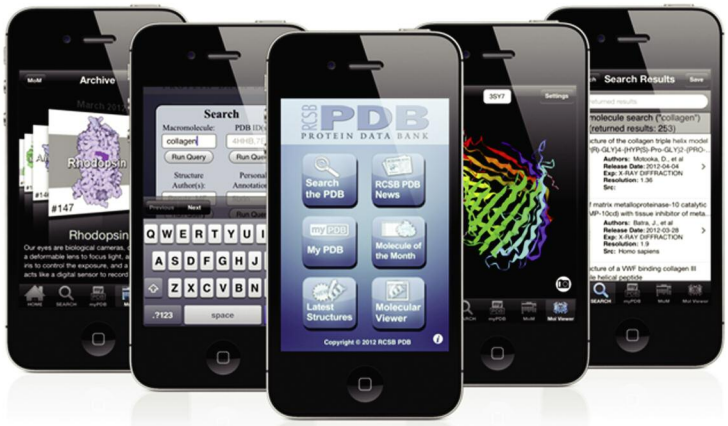
| | |
|---|---|
| 61940 | structure factors |
| 6794 | NMR restraints |
| 556 | NMR chemical shifts |

This newsletter is printed on recycled paper

# Message from the RCSB PDB

New and enhanced features have been added to the RCSB PDB, including:

**RCSB PDB *Mobile*.** Search the entire PDB, view the latest weekly release of structures, access your MyPDB account, view the entire catalog of *Molecule of the Month* articles, and more using either a WiFi or cellular data connection. RCSB PDB Mobile is an update of the beta-tested PDB*Mobile*.




*Access the free download of RCSB PDB Mobile from Apple's App Store.*

**Author Profiles.** This new PDB-101 feature displays a vertical timeline of the structures that list a particular researcher as a Deposition Author or Primary Citation Author. To jump to a specific time period, select a year from the right navigation menu or scroll down the page to load subsequent years.

**Query and Display Features**. Quickly search by Experimental and/or Molecule Type; view details about any revisions made to an entry from the Structure Summary page; and access Other Search Suggestions for top bar queries.

The **What's New** page has complete descriptions of all new features.


*Author Profile for J. Deisenhofer*

# Data Deposition and Annotation

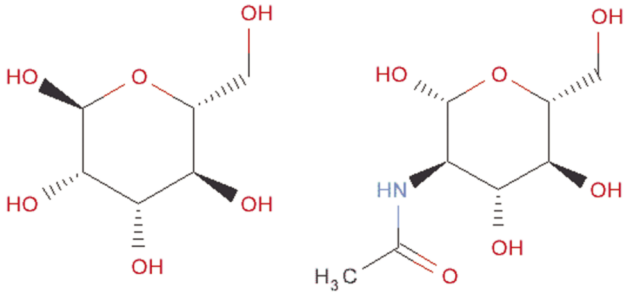
## Depositing Structures with Ligands

Ligand Expo (ligand-expo.rcsb.org) accesses chemical and structural information about all small molecule components found in PDB entries. It is based upon the Chemical Component Dictionary maintained by the wwPDB. When depositing a structure with a ligand:

- Search Ligand Expo for a chemical component that matches your ligand – If a match is found, use the corresponding three-character code for the ligand in your coordinates
- If the ligand is new, choose a new three-character code for the ligand
- When depositing your structure with ADIT, upload the chemical name and formula and/or a file showing the chemical image for the new ligand into the Ligand Information section

Ligand Expo can search the Chemical Component Dictionary using uploaded data files (e.g., PDB, MOL/SDF, Refmac/Phenix monomer library (mmCIF)); chemical name; formula; SMILES string; and ID code.

Searches for instances of ligands associated with macromolecular structures can also be performed at www.rcsb.org using a variety of options, including the top bar Chemical Name/ID search, Advanced Search, and the Chemical Structure Search. Users can then explore the ligand structures and the related PDB entries. Online screencasts are available at the RCSB PDB site to help users explore these features.




*Ligand Expo can also be used to check and confirm the chemistry of a chemical component. Shown is the correct sterochemistry for alpha-D-mannose (on the left, ID: MAN) and for N-acetyl-D-glucosamine (on the right, ID: NAG).*

## Deposition Statistics

From April 1-June 30, 2012, 2506 experimentally-determined structures were deposited to the PDB archive, and then processed and annotated by wwPDB teams.

Of the 4978 structures deposited in the first half of 2012 (January 1-June 30), 80% were deposited with a release status of "hold until publication"; 15% were released as soon as annotation of the entry was complete; and 5% were held until a particular date. 93% of these entries were determined by X-ray crystallographic methods; 6% were determined by NMR methods.

During the same time period, 4520 structures were released and made publicly available in the PDB.

## wwPDB News

### wwPDB News: *Journal of Biological Chemistry* to Require Validation Reports for Structure Papers

By the end of Summer 2012, *The Journal of Biological Chemistry (JBC)* will require authors to submit a validation summary report along with manuscripts describing X-ray crystallographic structure studies.

Validation reports are already required by the International Union of Crystallography (IUCr) journals as part of their submission process.

wwPDB members currently provide depositors with detailed reports that include the results of geometric and experimental data checking as part of the structure annotation process. These documents are available from all wwPDB annotation sites as PDF files for easy sharing and review.

The validation reports will continue to be developed and improved as we receive recommendations from our Validation Task Forces for X-ray,[1] NMR, EM,[2] and small angle scattering methods, and as we further develop our data deposition and processing procedures and the wwPDB Common Deposition & Annotation Tool.

More information about *JBC*'s announcement can be found at *ASBMB Today* (bit.ly/MKRDoc)

# Data Query, Reporting, and Access

## Tour the PDB with Drill-down Pie Charts

Standard characteristics of PDB entries—resolution, release date, experimental method, polymer type, organism, taxonomy—are used to create searchable data distribution summaries.

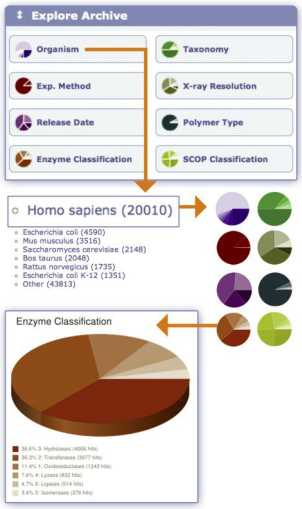
The *Explore Archive* widget on the home page provides a quick statistical overview of the PDB. Browse the charts individually, or view them all together by clicking on the "Show all" link. Clicking on a pie chart image will display a more detailed graphic that lists the percentages for the categories shown. Selecting one of the listed results will launch the corresponding structures in the Query Results Browser.

Data Distributions also appear at the top of the Query Results Browser, and can be used to view a quick statistical overview and to refine the results into subsets of interest. For example, users can "drill down" through these faceted search options to quickly access high

1. R. J. Read, P. D. Adams, W. B. Arendall, III, A. T. Brunger, P. Emsley, R. P. Joosten, G. J. Kleywegt, E. B. Krissinel, T. Lutteke, Z. Otwinowski, A. Perrakis, J. S. Richardson, W. H. Sheffler, J. L. Smith, I. J. Tickle, G. Vriend, P. H. Zwart (2011) A new generation of crystallographic validation tools for the Protein Data Bank. *Structure* **19**: 1395-1412.

2. R. Henderson, A. Sali, M. L. Baker, B. Carragher, B. Devkota, K. H. Downing, E. H. Egelman, Z. Feng, J. Frank, N. Grigorieff, W. Jiang, S. J. Ludtke, O. Medalia, P. A. Penczek, P. B. Rosenthal, M. G. Rossmann, M. F. Schmid, G. F. Schroder, A. C. Steven, D. L. Stokes, J. D. Westbrook, W. Wriggers, H. Yang, J. Young, H. M. Berman, W. Chiu, G. J. Kleywegt, C. L. Lawson (2012) Outcome of the first electron microscopy validation task force meeting. *Structure* **20**: 205-214.

resolution entries from a structure type search; human-related entries from a sequence search; or most recent entries returned from a chemical component search for a particular ligand. Any combination of categories is possible.




These charts can be hidden from the query results for users who want to only view the individual entries.

Data distribution summaries can also be used to explore the latest weekly update of PDB entries.

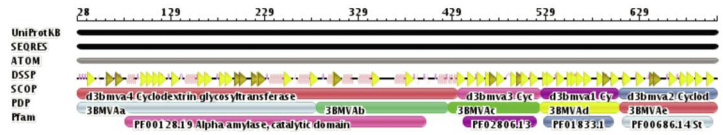
*Users can tour the PDB archive by drilling down on significant properties of structures such as Organism and Polymer Type with just a few clicks. This example shows the path to the EC distribution of structures from humans. Clicking on any link returns the structures that match all selected parameters. This feature is available to navigate through all search results and for the entire PDB archive.*

## Domain-based Structural Alignments

To provide more accurate results, the latest version of the 3D Similarity tab uses domain-based protein structure alignments instead of chain-based alignments.

For an example, see the 3D Similarity tab for glucanotransferase (PDB ID 3BMV).

An image of the sequence highlights how the residues listed in the sequence (SEQRES) and in the atom records (ATOM) map onto the relevant parts of the UniProtKB sequence, along with annotations from DSSP, SCOP, PDP and Pfam.

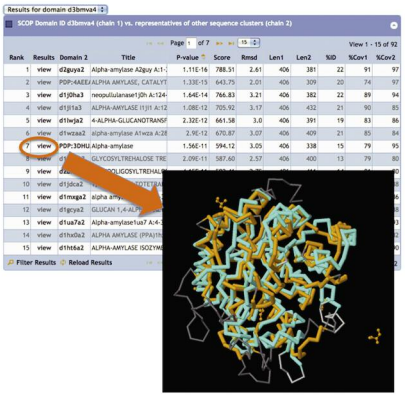



*The sequence diagram for PDB ID 3BMV[3] shows the corresponding UniProtKB sequence, the SEQRES and ATOM records, and the various annotations that are available.*

Domains are also highlighted in a table that displays the most important calculated results and scores. Domains can be selected from the pull-down menu above the table, or by clicking on a domain in the sequence image.

The table can be sorted and filtered, and offers links to a 3D structure alignment in Jmol (from the results column) and to information about similar domains. In the example of the 3D Similarity tab for 3BMV, selecting "view" for the domain PDP:3DHUAa launches the structure alignment view for the alpha amylase domains of 3BMV and 3DHU. Selecting the link for PDP:3DHUAa under the column Domain 2 returns the 3D Similarity tab for entry 3DHU.[4]

The calculation of the domain-split representative is an extension of our sequence clustering approach (see bit.ly/LvzUOo). To remove redundancy, we start with a 40% sequence identity clustering procedure, and select a representative chain from each sequence cluster. If the representative chain contains multiple domains, each is included. SCOP 1.75 domain assignments[5] are used when available. Otherwise, the assignments are computed using ProteinDomainParser.[6]




*In the example of the 3D Similarity tab for 3BMV, selecting "view" for the 7th-ranked domain PDP:3DHUAa launches the structure alignment view for the alpha amylase domains of 3BMV and 3DHU.[4] Selecting the link for PDP:3DHUAa under the column Domain 2 returns the 3D Similarity tab for entry 3DHU.*

## Bookmark and Post Webpages

Users can easily send and store RCSB PDB web pages using the "Share this Page" button.

With this service, favorite PDB entries, *Molecule of the Month* articles, and other features can be easily emailed to colleagues or posted to Facebook, Twitter, and LinkedIn.

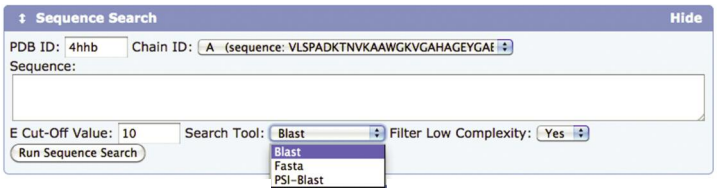

*Share this Page options.*

## Customized Home Page: Sequence Search

The RCSB PDB homepage is comprised of web widgets that can be moved around, minimized, or hidden so users can create a website that reflects their interests. Frequently-used features can be moved to the top, while less popular items can be hidden or collapsed.

The Sequence Search widget can search for a given sequence or a particular chain of any PDB entry using BLAST, FASTA, or PSI-BLAST. Options include specifying the E cut-off value and filtering low complexity.

To add this widget to your home page, select the Customize This Page button from the left menu. Download Files, Structure Comparison, and ADIT Deposition widgets can also be added.




*The **Search Sequence** widget. Enter a PDB ID to select a chain, or enter a sequence.*


3. R. M. Kelly, H. Leemhuis, H. J. Rozeboom, N. van Oosterwijk, B. W. Dijkstra, L. Dijkhuizen (2008) Elimination of competing hydrolysis and coupling side reactions of a cyclodextrin glucanotransferase by directed evolution. *Biochem J* **413**: 517-525.

4. J. B. Bonanno, M. Dickey, K.T. Bain, M. Iizuka, S. Ozyurt, D. Smith, S. Wasserman, J.M. Sauder, S.K. Burley, S.C. Almo (2008) *Crystal structure of an alpha-amylase from* Lactobacillus plantarum. **DOI: 10.2210/pdb2213dhu/pdb**.

5. A. G. Murzin, S. E. Brenner, T. Hubbard, C. Chothia (1995) SCOP: a structural classification of proteins database for the investigation of sequences and structures. *J Mol Biol.* **247**: 536-540.

6. N. Alexandrov, I. Shindyalov (2003) PDP: protein domain parser. *Bioinformatics* **19**: 429-430.

## Create a Collage of Structures

Different types of reports can be generated for a set of PDB entries, including the option to generate a collage of molecular images.

To create a collage, search for a group of structures, pull down the Generate Reports menu and select Custom Report>Image Collage. The query results will appear as a series of tiled molecular pictures.

Mousing over each image in the collage displays the structure title; clicking on the small image shows a larger version. The PDB ID listed links to the corresponding Structure Summary page.

Image collages can be customized by the size of the images displayed and how many images are shown per page.

Other Generate Reports options include creating customized tables or viewing pre-generated summary reports about structure, sequence, ligand, Structural Genomics Center, primary citation, and biological details.


*Image collage of virus structures.*

## Website Statistics

Access statistics for the second quarter of 2012 are shown.

| Month | Unique Visitors | Number of Visits | Bandwidth |
|---|---|---|---|
| APRIL | 258130 | 617748 | 778.90 GB |
| MAY | 244865 | 615509 | 794.33 GB |
| JUNE | 206864 | 525815 | 624.38 GB |

# Outreach and Education

## *Molecule of the Month* Reaches 150

June's article on Sliding Clamps is the 150th *Molecule of the Month* installment. With descriptions of structures from AAA+ proteases to zinc fingers, *Molecule of the Month* provides an easy introduction to macromolecular structures and the PDB archive. A slideshow highlighting other milestones is available online.

Written and illustrated since January 2000 by David S. Goodsell (The Scripps Research Institute), each entry links to high resolution illustrations, suggests topics for further exploration, and hosts customized, interactive 3D molecular views. Specific structures are highlighted each month in the article, and shown in specific PDB-101 views of individual structures.

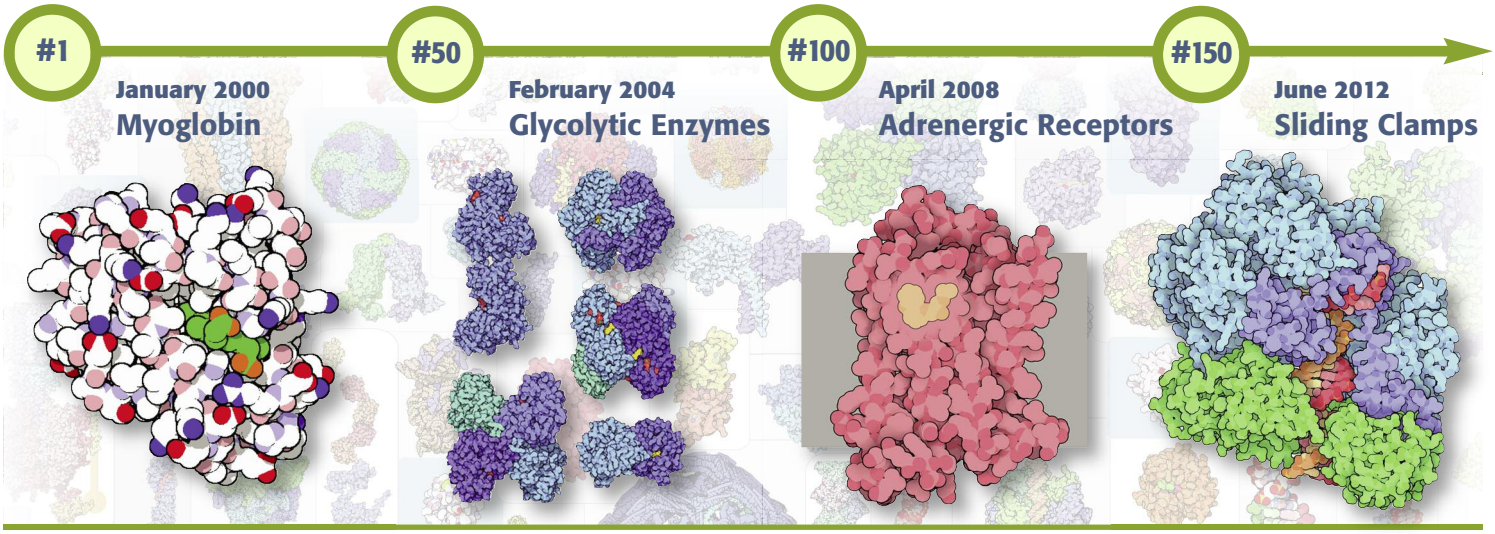
As the keystone of the PDB-101 educational resource, the *Molecule of the Month* supports teachers and students at all levels in their exploration of biology at a structural level.

PDB-101 supports different ways of exploring the *Molecule of the Month*, including:

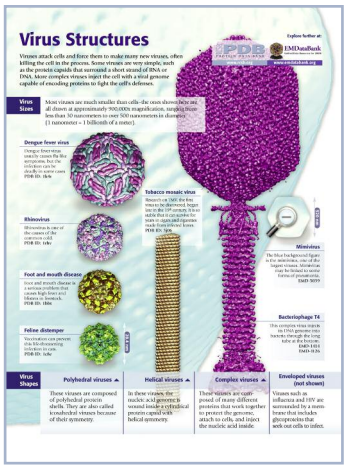
- **Quick alphabetical pulldown menu.** Jump from cholera toxin to influenza neuramindidase to anthrax toxin
- **Structural View of Biology interface.** Start with key topic categories and subcategories to drill down to individual articles and molecule examples. From the Biological Energy category, for example, users can select the subcategory Capturing the Energy in Food to find articles about structures such as pepsin, an enzyme that digests proteins. Then explore specific examples of pepsin and pepsinogen found in PDB entries 5pep and 3psg
- Archive of *Molecule of the Month* features organized by **Title, Date, and Category**, with links to individual PDF and ePub versions

*Molecule of the Month* articles are also available from the main RCSB PDB home page, top bar searches, structure search results, and individual Structure Summary pages.

Have suggestions for future *Molecule of the Month* columns? Let us know at info@rcsb.org!



## New Poster: *Virus Structures*




Learn about polyhedral, helical, complex, and enveloped viruses with examples drawn at approximately 900,000x magnification with a new poster that focuses on the shapes and sizes of different virus structures.

Structures from the feline distemper virus to mimivirus are highlighted.

*Virus Structures* joins other posters that illustrate *The Structural Biology of HIV*, *Molecular Machinery*, *How Do Drugs Work*, *Ribosome*, and *Toll-like Receptors*. Download them all from PDB-101.

PDB-101 also offers virus-related lesson plans and a template to fold a model of the dengue virus.

*Virus Structures* was created by the RCSB PDB and the EMDataBank.

## Meetings and Events

RCSB PDB participated in a variety of community events, including the San Diego Festival of Science and Engineering's Expo Day (March 24), UCSD's Triton Day (April 7), and Rutgers Day (April 28). Activities ranged from building DNA and viruses out of marshmallows to exploration of the RCSB PDB resource.

Curators and developers of biological databases convened at the **Fifth International Biocuration Conference** (April 2-4, Washington, DC) that was hosted by The Protein Information Resource (PIR). RCSB PDB's Lead Biocurator Jasmine Young co-chaired a session on *Protein structure, complexes, interactions* with Sona Vasudevan (PIR), and presented a poster on the *Worldwide Protein Data Bank: Current Projects*. Annotator Marina Zhuravleva gave a presentation on *Assessment of Structure-Model Quality and Validation of Macromolecular Structures at the Protein Data Bank*.

At the **Experimental Biology** meeting (April 21-25, San Diego, CA), the RCSB PDB met with researchers and educators at the exhibit booth. Attendees, particularly from the American Society for Biochemistry and Molecular Biology, were interested in the new searching and reporting features of the RCSB PDB website.

Director Helen Berman gave the keynote lecture for the **NJ Women in Science & Technology Workforce Summit** on June 15 (hosted by the NJ State Employment and Training Commission).

Upcoming meetings include:

**ISMB and 3Dsig**: This year, the International Society for Computational Biology is celebrating the 20th year of the ISMB–Intelligent Systems for Molecular Biology–conference (July 15-17. Long Beach, CA).

RCSB PDB Associate Director Phil Bourne was recently interviewed in the *Journal of Computer-Aided Molecular Design* (2012) **26**: 165-167, DOI: 10.1007/s10822-012-9555-0

Presentations will include *Internal pseudo-symmetry in proteins* (Andreas Prlić) and *Efficient searching and mining of the RCSB Protein Data Bank* (Peter Rose).

At the ISMB Special Interest Group meeting Bioinformatics Open Source Conference (BOSC), Andreas Prlić will also present *How to use BioJava to calculate one billion protein structure alignments at the RCSB PDB website*.

At the 3Dsig:Structural Bioinformatics & Computational Biophysics satellite meeting, John Westbrook will discuss *Format déjà vu: PDBX/MMCIF, the new data format for the wwPDB*. *Molecule of the Month* author David Goodsell will describe *Communicating and Interacting with the Molecular Cell* (along with Arthur Olson). Associate Director Phil Bourne is one of the 3Dsig Program Chairs.

The RCSB PDB Poster Prize will be awarded for the best student poster presentation in the category of *Structure and Function Prediction*.

**ACA**: At the Annual Meeting of American Crystallographic Association (July 28-August 1; Boston, MA), the RCSB PDB will be exhibiting alongside the Structural Biology Knowledgebase.

Director Helen Berman will present *Data Management of Small Molecule Ligands, Antibiotics, and Peptide Inhibitors in the PDB* during the session on Structure-Guided Drug Discovery. Lead Annotator Jasmine Young will give an update of *Current Projects of the Worldwide Protein Data Bank*.

David Goodsell will be participating in *Crystallography: World of Wonders*, a workshop that will provide high school teachers with the materials and knowledge needed to introduce crystallography to their classrooms.

The RCSB PDB Poster Prize will be awarded for the best student poster involving macromolecular crystallography.


*Expo Day, Rutgers Day, and Triton Day activities.*

**Protein Society**: Helen Berman is the 2012 Awardee of the Carl Brändén Award of the Protein Society (August 5-8; San Diego, CA). The Award, sponsored by the Rigaku Corporation, is given to an outstanding protein scientist who has also made exceptional contributions in the areas of education and/or service to the science.

During the Plenary Awards Session, she will present *Trendspotting from the Protein Data Bank*, which will look at different trends seen in the data archive, and what they might mean for the future of biology

## Congratulations to National Protein Modeling Champions

The National Science Olympiad Tournament was held May 18-19 at the University of Central Florida.

Teams built a model of MHC 1hsa, and brought along their prebuilt models of caspase protein 1i3o.

The top scoring teams in this event were:
1) New Trier High School (IL)
2) Troy High School (CA)
3) Camas High School (WA)

Protein modeling is managed by the MSOE Center for BioMolecular Modeling (CBM) and hosted in NJ by the RCSB PDB. This event will be on hiatus from the tournament for two years as other events are incorporated. The RCSB PDB's related Twitter account **@buildmodels** will continue to post education and PDB-related news and links.

*First place New Trier High School and MHC models. Images from CBM.*

# Education Corner by Andrew K. Vershon, Ph.D.

## The Waksman Student Scholars Program: Learning Science by Doing Science

**DR. ANDREW K. VERSHON** *is a Professor and Undergraduate Director in the Department of Molecular Biology and Biochemistry at the Rutgers University and the Director of the Waksman Student Scholars Program.*

*He also directs a research laboratory at the Waksman Institute, where the major focus of his research is on the regulation of transcription in the yeast* Saccharomyces cerevisiae.

*For more information about the Waksman Student Scholars Program, please visit* ***wssp.rutgers.edu*** *or contact Sue Coletta (coletta@waksman.rutgers.edu).*

The Waksman Student Scholars Program (WSSP) provides opportunities for high school students and their biology teachers to contribute to authentic research in molecular biology and bioinformatics.

Since July 1993, over 250 high school science teachers and approximately 5,000 high school students have participated in the project. The WSSP is a year-long program that begins with a summer Institute in which teachers and one or two of their students learn the background content, rationale, and methods required to conduct the research project. It continues during the academic year, when as many as 60 students from each school carry out the research at their own high schools. Schools select how the research project will be integrated into their existing curriculum structure, as either an independent research course, as part of an Advanced Placement (AP) Biology course, or as an after-school club. The program is currently being conducted at the Waksman Institute at Rutgers University, the Johns Hopkins University, the University of Texas at Austin, and the Lawrence Livermore National Laboratory in California. The WSSP and its affiliated programs receive support from the Waksman Institute, GE Healthcare Life Sciences and the National Science Foundation.

### Principles Guiding the Project

Over the last two decades the biological sciences have experienced a remarkable transformation. New technologies have produced a flood of information that has to be stored, linked, accessed, and distributed. A cyberinfrastructure in support of biology has become widespread,[7] and computers are now an essential tool in the biologists' repertoire. Yet, reports indicate that the K-12 curriculum has not reflected these changes.[8]

Evidence shows that students who engage in authentic research increase their understanding of scientific processes and change their perception about science.[9] Working with an open-ended, unsolved research problem affords students with the opportunity to "learn by doing." They can learn how to develop experimental designs, analyze data, devise and test models, and share ideas.[10] Students can also access Internet resources to work on research problems using the authentic data that they generate. The skills that students acquire by using online tools, navigating through professional websites, interpreting complex data, and reporting their findings, will be essential throughout their careers.[11]

A problem with using the scientific computational resources is that high school teachers and their students may be unfamiliar with some of the specialized content and the methodologies that are required

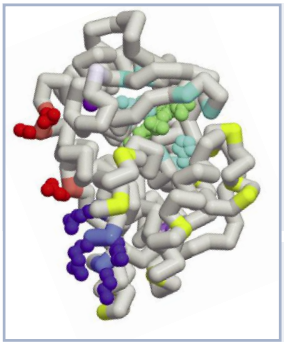


*Figure 1: A model of ascorbate peroxidase (1APX)[17] created by students from Bayonne High School, NJ. The heme group is shown in light green and the position of the side chains and backbone atoms that contact the heme are shown in aqua. The red and blue residues show negative and positive charged side chains, respectively, that form contacts along the dimer interface of the protein in the crystal structure. The yellow marks positions that are not conserved between the sequence of the protein determined from the gene the students isolated from the duckweed plant* Wolffia australiana *and the pea* Pisum sativum.

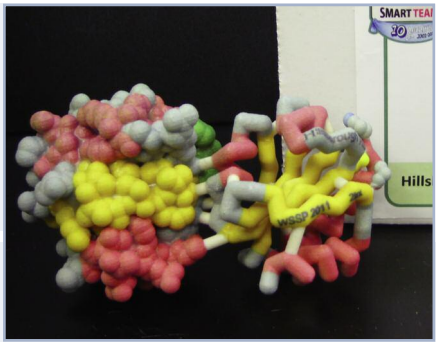



*Figure 2: A physical model of thioredoxin (2TRX)[18] created by the students of Hillsborough High School, NJ. A dimer is shown in which one monomer is displayed in spacefill and the other in backbone.*

to use these resources. However, there are many examples of individual high school teachers or students who successfully learn to use these scientific tools by working in a research laboratory. This raises the question of whether resources can be developed so that diverse populations of high school students can learn to use these tools to conduct authentic research and make genuine contributions to scientific knowledge.

To address this question, the WSSP has developed an authentic research project and accompanying software program that guides students through the analysis of novel DNA sequences to determine a) if they are similar to other sequences stored in the scientific databases, b) if they code for proteins, c) if so, what is the function of the proteins, and d) examine the 3D structures of homologs of these proteins. Students conducting the research project select random clones from a plasmid cDNA library provided by the WSSP, purify the plasmid DNA, determine the size of the DNA insert by agarose gel electrophoresis of restriction enzyme digests and polymerase chain reactions (PCR). The DNA sequences of the inserts are determined and students use an online program to evaluate the quality of the sequence data and resolve ambiguities. They search the online databases for similar DNA sequences and, where applicable, for the proteins that are coded by the DNA. The students use this information to investigate the likely function of the protein and determine if it is associated with a specific cellular process or disease. When analyzing the DNA sequence and protein structure data, students work with the same research tools that scientists use every day.

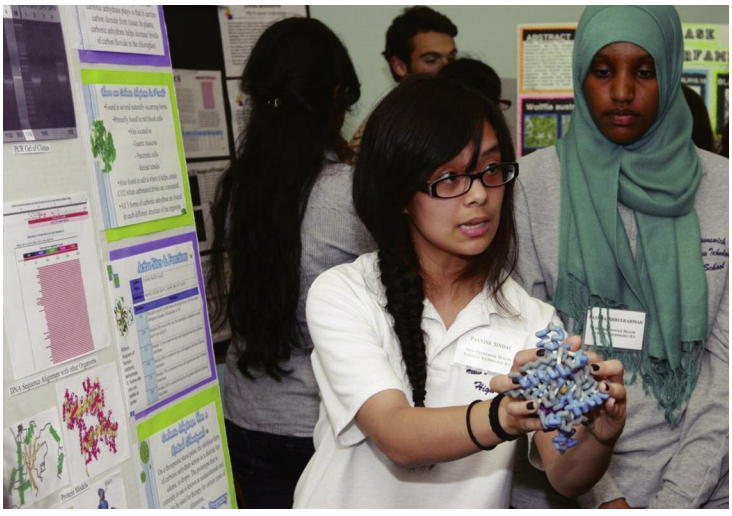


*Figure 3: Students from New Brunswick Health, Sciences, and Technology High School, NJ presenting their research on a homolog of carbonic anhydrase (1EKJ)[19] at the year-end WSSP Poster Forum.*

Each student has the opportunity to analyze a unique DNA sequence that has not been previously examined. They are therefore able to publish their findings on GenBank,[12] the DNA sequence database maintained by the National Center for Biotechnology Information (NCBI) and used by scientists throughout the world. The students are able to add to the body of scientific knowledge, and become part of a community of practice.

Most of the students' DNA sequences code for proteins that are similar to proteins in the PDB, in which the 3D structures have been determined. As part of the analysis of their DNA sequences, students examine the structures of these proteins using one of the many freely available molecular graphics programs, such as Jmol,[13] RCSB PDB's Simple Viewer,[14] or Cn3D.[15] Students view the secondary, tertiary and quaternary structures of the proteins, along with identifying active sites and important structural components. Some of the students extend the structural analysis by creating models in Jmol. After examining the primary citations associated with an entry, students design models that can show the active site residues, contact regions with other proteins, or other important structural features (Figures 1 and 2). Other students design models that highlight sequence identity and conservation between the protein they identified and the protein in the PDB. Through a collaboration with the Center for BioMolecular Modeling (**cbm.msoe.edu**) and as part of the HHMI-funded Students Modeling A Research Topic (SMART) Team project (see the Winter 2006 Education Corner),[16] it has been possible to obtain physical models of the proteins designed by students (Figure 2 and 3). By working with these modeling programs, students gain a deeper understanding of protein structure and function.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Web: www.rcsb.org
Email: info@rcsb.org
FTP: ftp.wwpdb.org

## RCSB PDB Partners

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

RUTGERS

Rutgers, The State University of New Jersey
Center for Integrative Proteomics Research
174 Frelinghuysen Road
Piscataway, NJ 08854-8087

UCSD SDSC • SKAGGS SCHOOL of PHARMACY and PHARMACEUTICAL SCIENCES

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

WORLDWIDE PDB PROTEIN DATA BANK

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

## RCSB PDB Management

**DR. HELEN M. BERMAN**, Director
Rutgers, The State University of New Jersey
berman@rcsb.rutgers.edu

**DR. MARTHA QUESADA**, Deputy Director
Rutgers, The State University of New Jersey
mquesada@rcsb.rutgers.edu

**DR. PHILIP E. BOURNE**, Associate Director
San Diego Supercomputer Center and the Skaggs School of Pharmacy and Pharmaceutical Sciences,
University of California, San Diego
bourne@sdsc.edu

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

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www.rcsb.org • info@rcsb.org
Rutgers, The State University of New Jersey
Center for Integrative Proteomics Research
174 Frelinghuysen Road
Piscataway, NJ 08854-8087
USA