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RCSB PDB
PROTEIN DATA BANK

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Research Collaboratory for Structural Bioinformatics Protein Data Bank

NEWSLETTER

www.pdb.org • info@rcsb.org

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

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DATA DEPOSITION AND ANNOTATION

DATA QUERY, REPORTING, AND ACCESS

OUTREACH AND EDUCATION

SNAPSHOT: OCTOBER 1, 2010

68,288 released atomic coordinate entries

MOLECULE TYPE		EXPERIMENTAL TECHNIQUE	
63,236	proteins, peptides, and viruses	59,210	X-ray
		8,596	NMR
2,173	nucleic acids	308	electron microscopy
2,841	protein/nucleic acid complexes	27	hybrid
38	other	147	other
		48,592	structure factor files
		5,891	NMR restraint files

This Newsletter is printed on recycled paper

Message from the RCSB PDB

The RCSB PDB's *Molecule of the Month* introduces readers to the structure and function of specific molecules, and shows how the structures function and their importance in our lives. Each entry is illustrated through descriptive text and pictures, with links to specific PDB entries, discussion questions, and interactive 3D molecular views. As of October 2010, there are now 130 articles describing everything from AAA+ proteases to zinc fingers.

These columns have been organized to help users explore the *Molecule of the Month*–and the PDB archive–in the context of biology. Major functional categories can be browsed by areas of interest. Within each topic, descriptive subcategories lead to the relevant *Molecule of the Month* features.

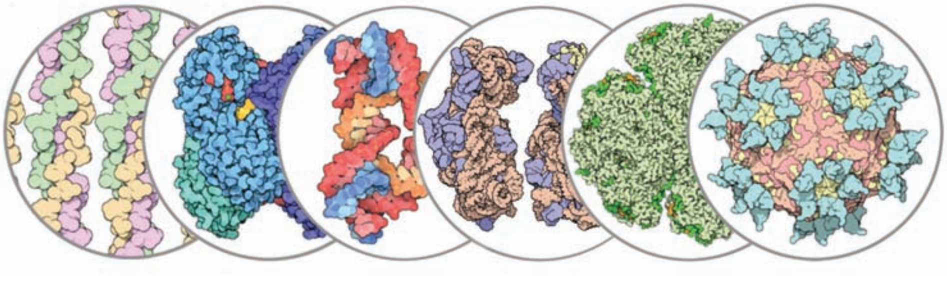
The major topic categories include:

- **Protein Synthesis**: including the major molecules of protein synthesis, from DNA to RNA to ribosomes to folded proteins.
- **Enzymes**: further organized enzyme class.
- **Health and Disease**: covers topics such as drug action, viruses, and the molecular basis of disease.
- **Biological Energy**: presents the processes for capturing and converting energy in cells.
- **Infrastructure and Communication**: includes topics such as structural proteins and cell signaling.
- **Biotechnology and Nanotechnology**: explores the ways scientists look to nature for inspiration, and harnessing biological machinery for use in science and technology.

Past *Molecule of the Month* articles can still be searched by date and feature title, but the category view lets users access the *Molecule of the Month* archive with a biological interest in mind, rather than a specific molecule. The **Biological Energy** topic category, for example, contains subcategories Capturing the Energy in Food, Photosynthesis, Molecular Motors, and Creating and Capturing Light. Each subcategory can then be browsed for the related *Molecule of the Month* features.

The same article will be listed under multiple categories/subcategories if it can be categorized in several ways.

We hope that this new interface will promote new ways of exploring these articles and the PDB archive.



Data Deposition and Annotation

New Release of pdb_extract Available Online and for Download

pdb_extract is a program that minimizes errors and saves time during the deposition process by extracting key details from the output files produced by many X-ray crystallographic and NMR applications. The program merges these data into macromolecular Crystallographic Information File (mmCIF) data files that can be used with ADIT for validation and deposition.

Version V3.10 of pdb_extract has been released, and provides

- Support for several new versions of programs (including REFMAC version 5.5 and higher), for a total of 37 programs/packages with hundreds of different formats
- Improved extraction and parsing from programs (e.g., PHENIX version 1.4 and later, BUSTER-TNT version 2.8 and higher) and log files (MLPHARE)
- Support for multiple MTZ file conversion

At pdb-extract.rcsb.org, depositors can upload files into the webserver or download the latest workstation version. Complete details are available in the online release notes and manual. Tutorials are also available for X-ray and NMR.

Redesigned BioSync

The structural biologist's online guide to high energy data collection facilities has been enhanced with a new layout and features.

BioSync (biosync.sbkb.org) is the structural biologist's online guide to high energy data collection facilities. As data collected from synchrotron beamlines currently account for more than 80% of all X-ray crystallographic entries deposited to the PDB, the BioSync resource has been upgraded with a new layout and features. BioSync provides detailed information and usage statistics for macromolecular beamlines at synchrotron facilities worldwide.

To explore BioSync, select one of the options from the top menu bar:

- Information about each synchrotron is organized by location. Data sheets for operational macromolecular beamlines at synchrotrons worldwide describe available services and functions (new data additions include remote data collection; mail-in, crystallization and structure solution services; robotics handling for crystal screening and mounting; microfocus beams and facilities for collecting data under extreme conditions). Users can also search for specific capabilities, services and equipment across beamlines. Beamline information is uploaded by synchrotron personnel.

- Deposition statistics are grouped by synchrotron and by geographical region. Site statistics are broken down to the beamline level; new graphs compare beamlines within a site. Galleries of structures and tables containing citations and other general information (e.g., phasing methods, wavelength used for data collection, resolution, R-factors, numbers of atoms) are also available. A separate set of statistical tables, galleries and informational tables is provided for structures produced by structural genomics efforts.

- Simple and Advanced Search options are available. Simple searches look for synchrotrons by name or location; a new feature can return a breakdown of structure counts per country for a site or a single beamline. The Advanced Search can be used to look for more detailed beamline features and services.

The redesign and upgrade of BioSync was funded by NIGMS. Questions? Email biosync@sbkb.org.

PSI | nature StructuralBiology Knowledgebase

Structural Genomics in the News

Form and Function Targeted by PSI:Biology

The National Institutes of Health have awarded 23 grants for structural biology research totaling up to $290 million over 5 years. Four high-throughput centers, nine membrane protein centers, and ten biological partners to these centers will be funded to focus on human disease and biological processes. For full news: www.nigms.nih.gov/News/Results/20100930.htm

PSI:Biology continues to invite biologists to join their multinational structure determination efforts. For more information: grants.nih.gov/grants/guide/pa-files/PAR-10-214.html

Introducing the Revamped Structural Biology Knowledgebase

In line with the recent launch of the PSI:Biology program, the Structural Genomics Knowledgebase became the **Structural Biology Knowledgebase** in September. The site has been reorganized to better support users' interest in targets, methods, structure-sequence-function, and theoretical models.

The October SBKB update published the final articles in a series highlighting the progress made by the PSI over the past decade in the areas of methods, models, structures, and outreach. Access these articles and new features at sbkb.org.

Journal Highlights JCSG Accomplishments

The Joint Center for Structural Genomics (JCSG) has published a special open access issue of Acta Crystallographica Section F with more than 30 articles covering high throughput technology, domains of unknown function, new folds, fold variants, the human gut microbiome, functional characterization with ligands, and NMR methods development. Read the issue at journals.iucr.org/f/issues/2010/10/00/issconts.html

SGC Celebrates its 1000th Deposited Structure

The Structural Genomics Consortium (SGC) recently deposited a milestone 1000th structure into the PDB. Entry 2xml is a 'gene switch' protein involved in epigenetic signaling.

SGC is a multinational public-private partnership that focuses on biomedically important targets from the human proteome. For full news: www.thesgc.org/news/1000th_structure

Deposition Statistics

In the third quarter of 2010, 2310 experimentally-determined structures were deposited to the PDB archive. The entries were processed and annotated by wwPDB teams at the RCSB PDB, PDBe, and PDBj.

Of the structures deposited, 78.3% were deposited with a release status of "hold until publication"; 3.0% were released as soon as annotation of the entry was complete; and 18.7% were held until a particular date. 93.1 % of these entries were determined by X-ray crystallographic methods; 6.2 % were determined by NMR methods.

During the same time period, 2097 structures were released in the PDB, for a total of 6142 structures released in 2010.

wwPDB News from wwpdb.org

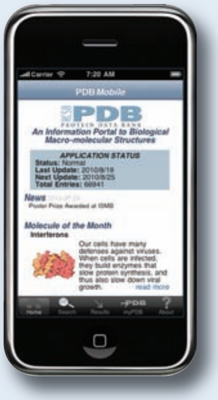
Get the Latest wwPDB News

Subscribe to the wwPDB RSS (Really Simple Syndication) Feed to get the news related to the wwPDB as it is published. This feed pushes information to RSS readers so users can easily keep up to date with wwPDB announcements.

The wwPDB website (wwpdb.org) posts announcements relating to policy, distribution, and events. Recently, the wwPDB has announced a requirement of Chemical Shift Data for deposition, the availability of Validation Reports for sharing with journal review editors, and the addition of Version 2 NMR Restraint Files to the wwPDB FTP.

Data Query, Reporting, and Access

Latest Website Release



An Information Portal to Biological Macro-molecular Structures

APPLICATION STATUS
Status: Normal
Last Update: 2010/8/18
Next Update: 2010/8/25
Total Entries: 68941

News
Poster Prize Awarded at ISMB

Molecule of the Month
Interferons

Our cells have many defenses against viruses. When cells are infected, they build enzymes that slow protein synthesis, and thus also slow down viral growth. read more

To install PDBMobile on your iPhone or iPod (with at least iOS 4.1), point its web browser to www.pdb.org.

New and enhanced features were added to www.pdb.org at the beginning of October, including:

• **Improved navigation of the *Molecule of the Month* archive**: new category views and a new sortable table to view features by category, date and name.

• **PDBMobile for the iPhone**: search the RCSB PDB, browse results, access MyPDB, and read the latest news and *Molecule of the Month* features.

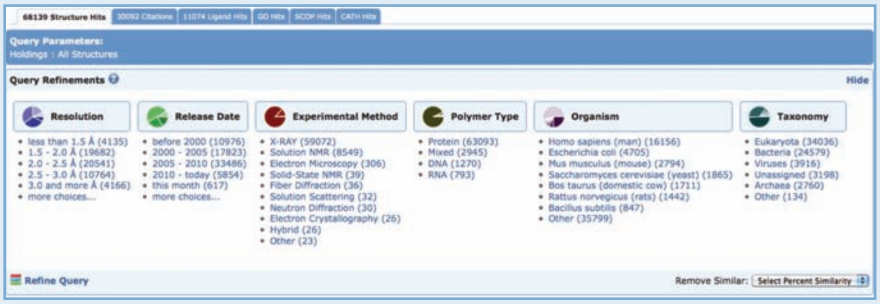
PDBMobile is an HTML5-based application for mobile devices. It initially targets iPhone and iPod devices running iOS4. Future releases will target other platforms, including the iPad, Google Android and Windows Phone 7.

• New ways to explore search results using **data distribution summaries**. Search results now offer summary charts for standard characteristics of PDB entries (resolution, release date, experimental method, polymer type, organism, taxonomy) that can be used to refine search results into subsets of interest. For example, users can use these drill-down options, or 'faceted search' options, to quickly access high resolution entries from a structure type search; human-related entries from a sequence search; or most recent entries resulting from a chemical component search. Any combination of categories is possible.

• **Integration with Binding Affinity Data from BindingDB** (www.bindingdb.org). The Ligand Chemical Component widget on a Structure Summary page lists and links to binding affinity data from BindingDB (when available).

• **New Help features**, including a sitemap and glossary.

For complete descriptions, see the **New Features** widget on the RCSB PDB home page.



Query Parameters:
Holdings : All Structures

Query Refinements

Resolution
- less than 1.5 Å (4135)
- 1.5 - 2.0 Å (19682)
- 2.0 - 2.5 Å (20541)
- 2.5 - 3.0 Å (10764)
- 3.0 and more Å (4166)
- more choices...

Release Date
- before 2000 (10976)
- 2000 - 2005 (17823)
- 2005 - 2010 (33486)
- 2010 - today (5854)
- this month (617)
- more choices...

Experimental Method
- X-RAY (59072)
- Solution NMR (8549)
- Electron Microscopy (306)
- Solid-State NMR (39)
- Fiber Diffraction (36)
- Solution Scattering (32)
- Neutron Diffraction (30)
- Electron Crystallography (26)
- Hybrid (26)
- Other (23)

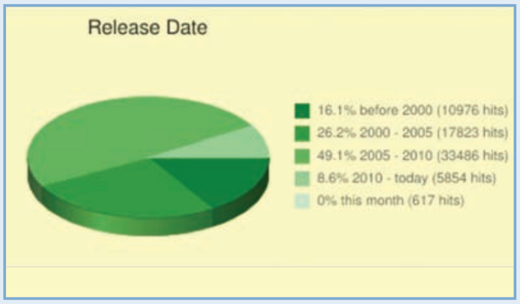
Polymer Type
- Protein (63093)
- Mixed (2945)
- DNA (1270)
- RNA (793)

Organism
- Homo sapiens (man) (16156)
- Escherichia coli (4705)
- Mus musculus (mouse) (2794)
- Saccharomyces cerevisiae (yeast) (1865)
- Bos taurus (domestic cow) (1711)
- Rattus norvegicus (rats) (1442)
- Bacillus subtilis (847)
- Other (35799)

Taxonomy
- Eukaryota (34036)
- Bacteria (24579)
- Viruses (3916)
- Unassigned (3198)
- Archaea (2760)
- Other (134)

Remove Similar:

Data distribution summaries can be used to explore the latest weekly update of PDB entries or the entire PDB archive by clicking on the links in the top menu bar (In this example, it read As of Tuesday Sep 21, 2010 at 5 PM PDT there are 68139 Structures*).*



Each chart can be used to drill down further, or to explore the entries in a given data distribution.

Analyze Small Molecule Interactions in the PDB with Ligand Explorer

Ligand Explorer can display hydrogen bonds, hydrophobic interactions, bridged H-bonds, metal interactions, and neighboring residue interactions and thresholds in a dynamic viewer.

Users can toggle interactions on/off, adjust distance thresholds, label interactions by distance, and display all neighbor residues. Distances, angles, and dihedral angles can be analyzed and measured. The views created can be saved as an image file, or as a text file listing interactions.

Ligand Explorer can be accessed from the Ligand Chemical Component section of an entry's Structure Summary page. The program uses the same Molecular Biology Toolkit[1] as the RCSB PDB's Protein Workshop and Simple Viewer.

Launching Ligand Explorer can install a local copy of the program on your computer, and can be used to read a local PDB file, or access a PDB file directly using the File menu (when online).

Structure: 2W70

☑ Hydrogen Bond 3.3
☐ Hydrophobic 3.9
☑ Bridged H-Bond 3.3
☐ Metal Interaction 3.5
☐ Neighbor Residues 4.0
☑ Label interactions by distance

Ligand Explorer dynamically displays the interactions in PDB entry 2w70[2]

Website Statistics

Website access statistics for second quarter of 2010 are given below.

Month	Unique Visitors	Number of Visits	Bandwidth
JUL 2010	154256	395745	767.18 GB
AUG 2010	159350	396199	783.32 GB
SEPT 2010	201919	477825	1344.88 GB

dConsensus

A paper describing dConsensus has been published:

dConsensus: a tool for displaying domain assignments by multiple structure-based algorithms and for construction of a consensus assignment. Kieran Alden, Stella Veretnik, Philip E Bourne (2010) *BMC Bioinformatics* **11**:310. **doi:10.1186/1471-2105-11-310**

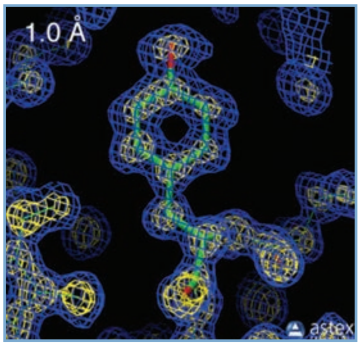
Outreach and Education

Tools for Education

The RCSB PDB offers resources for teachers and students; many are described in the recently-published *Promoting a structural view of biology for varied audiences: an overview of RCSB PDB resources and experiences* (S. Dutta, C. Zardecki, D. S. Goodsell, H. M. Berman (2010) *J. Appl. Cryst.* **43**: 1224-1229 doi:10.1107/S002188981002371X).

Accessible from the left hand menu, the RCSB PDB's Education section offers:

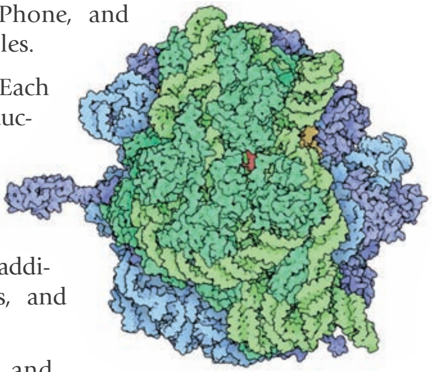
- **Understanding PDB Data**: Through text, images, and interactive Jmols, this feature intends to help researchers and educators get the most out of the PDB archive. Broad topics include how to understand PDB data, how to visualize structures, how to read coordinate files, and potential challenges in exploring the archive.



The use of electron density maps in determining molecular structure is described in the online resource Understanding PDB Data.

- **Educational Resources**: Many of the educational materials created by the RCSB PDB, including animations and handouts, are archived here. Recent additions include an updated edition of the *Bioinformatics of Green Fluorescent Protein* tutorial guide and the *How Do Drugs Work?* poster and flyer.
- RCSB PDB Newsletters and *Education Corner*: Each quarter, new developments, outreach efforts, and interviews with leaders in the community are published in an online and printed newsletter. Each *Education Corner* column, which highlights PDB usage in the classroom, has been archived on a single page. Past *Education Corners* have featured a rubric for biomacromolecular 3D literacy, the program *Molecules* for the iPhone, and physical 3D models of molecules.
- ***Molecule of the Month***: Each installment includes an introduction to the structure and function of a particular molecule, a discussion of the relevance of the molecule to human health and welfare, suggested additional readings and resources, and interactive views.

To illustrate the features and functionality of the RCSB PDB website, online screencasts provide short guides to selected features. A more detailed tutorial is also available at **openhelix.com**.



The Molecule of the Month feature on 70S ribosomes discusses the process of protein synthesis. Other popular editions focus on green fluorescent protein, tobacco mosaic virus, and DNA.

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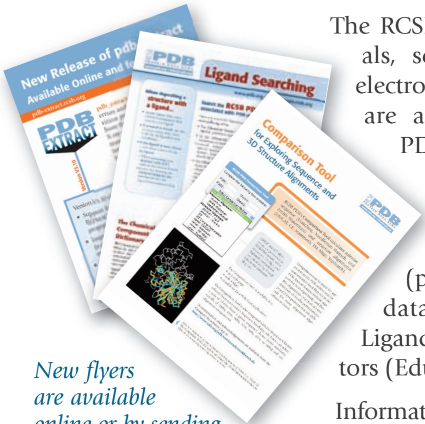
[1] The Molecular Biology Toolkit (MBT): A Modular Platform for Developing Molecular Visualization Applications (2005) *BMC Bioinformatics*, **6**: 21. [2] Mochalkin et al. Discovery of antibacterial biotin carboxylase inhibitors by virtual screening and fragment-based approaches (2009) *ACS Chem.Biol.* 4: 473–483.

New Flyers Available



New flyers are available online or by sending a request to ***info@rcsb.org****.*

The RCSB PDB publishes news, tutorials, screencasts, guides, and more electronically. New printed materials are also distributed at the RCSB PDB's exhibit booths at professional society meetings.

These flyers describe resources of interest to data depositors (pdb_extract, sugar geometry), data users (Comparison Tool, Ligand Searching, Widgets), educators (Educational Resources) and more.

Information is also available about related resources, including the wwPDB (Validation Reports and RSS Feed), the new version of the BioSync Guide to Synchrotron Facilities, and the Electron Microscopy Data Bank.

For a customized packet of flyers and information for your lab or department, please send your postal address and user type (depositor, users, educator, all) to **info@rcsb.org**.

Poster Prizes Awarded

The RCSB PDB awards a poster prize for the best student poster presentation at a number of different meetings throughout the year. For more information about the award, please see **www.pdb.org**.

Poster Prize Winner at ISMB: Mickey Kosloff

At the 18th Annual International Conference for **Intelligent Systems for Molecular Biology** (ISMB, July 11-13; Boston, MA), the award for best student poster in the category of Structure and Function Prediction went to Mickey Kosloff *for Structure-based redesign of selective G-protein inactivation by RGS proteins* (Mickey Kosloff, Amanda M. Travis, Vadim Y. Arshavsky, Duke University Medical Center).

Many thanks to the judges: Manisha Brahmachary, Brian Chen, Fabian Dey, Markus Fischer, Tobias Hamp, Laszlo Kajan, Eugenia Lyashenko, Marco Punta, Shruti Rastogi, Ta-tsen Soong (Columbia University), Avner Schlessinger (University of California San Francisco), and Mikhail Dozmorov (Oklahoma Medical Research Foundation). Thanks also to Poster Committee Chair Yana Bromberg (Columbia University) and to the International Society for Computational Biology.

At the 2010 Meeting of the **American Crystallographic Association** (ACA, July 24-29; Chicago, IL), the award went to Serah Kimani for *Catalysis in the nitrilase superfamily amidases: Insights from the active site* (Serah Kimani[1], Brandon Weber[2], Andrew Nel[3], Don Cowan[3], Trevor Sewell[2]. [1]Molecular and Cell Biology Department, University of Cape Town, [2]Electron Microscope Unit, University of Cape Town, [3]Department of Biotechnology, University of the Western Cape). Serah also won the award in 2007.

Honorable mentions were made to Yuan Cheng (*A uniquely open conformation revealed in the structure of a novel protein arginine Methyltransferase*, Yuan Cheng, Monica Frazier, Matthew Redinbo, University of North Carolina at Chapel Hill) and Jennifer Cash (*The structure of the muscle growth inhibitor myostatin bound to follistatin 288: Insights into receptor utilization and heparin binding*, Jennifer Cash[1], Carlis Rejon[2], Alexandra McPherron[3], Daniel Bernard[2], Thomas Thompson[1]. [1]University of Cincinnati, [2]McGill University, [3]National Institutes of Health).

Marina Zhuravleva (RCSB PDB), Yuan Cheng, Michael James, Serah Kimani, and Jennifer Cash at the ACA Banquet & Award Ceremony.

Many thanks to the ACA judges: Michael James (University of Alberta), Cheryl Klein Stevens (Xavier University), Bi-Cheng Wang (University of Georgia), Eric Ortlund (Emory University), and Charles Carter (University of North Carolina at Chapel Hill). Thanks also to Poster Committee Chair Victor G. Young, Jr. (University of Minnesota) and to Marcia Colquhoun and the ACA.

Sven Dahms

Sven Dahms received the poster prize at the 26th **European Crystallographic Meeting** held in Darmstadt, Germany (August 29 - Sept 2) for *Structure and biochemistry of the APP E2-domain* (Sven O. Dahms, Dirk Roeser, Manuel E. Than, Fritz Lipmann Institute, Jena, Germany).

Many thanks to the judges: Wolf-Dieter Schubert (Helmholtz Centre for Infection Research) and Norbert Straeter (University of Leipzig), and to Andreas Roodt, Petra Bombicz, and the European Crystallographic Association.

Recent Meetings and Presentations

In addition to the poster prize award, the RCSB PDB exhibited alongside the PSI SBKB at the **ISMB** meeting. At the 3DSIG satellite meeting on Structural Bioinformatics and Computational Biophysics, Andreas Prlić presented *New RCSB PDB protein comparison tools for sequence and 3D structure*.

At the **ACA** meeting, other activities included

- The *Molecule of the Month's* David Goodsell participated in the ACA's workshop for high school teachers called *Crystallography: World of Wonders*.
- A PDB Depositors' Lunch updated users on the wwPDB Common Deposition and Annotation Tool project and collect feedback.
- A poster described the *wwPDB Common Annotation and Deposition Tool Development*.

Visitors to the RCSB PDB/PSI SBKB booth at ACA learned about new features such as wwPDB Validation PDFs, the latest version of pdb_extract, the Comparison Tool for sequence and structure, and much more.

David Goodsell presented *Getting the most out of the Protein Data Bank* at the Educator's Luncheon Workshop at The 24th **Annual Symposium of the Protein Society** (August 1-5; San Diego, CA). Also at this meeting, Andreas Prlić presented a poster entitled *Detection of remote similarities in protein structures in the RCSB PDB* that illustrated the functionality of the RCSB PDB's Comparison Tool.

Several events happened at the **American Chemical Society**'s Fall National Meeting (August 22-26, Boston, MA). At the *PDB and Chemistry* symposium, presenters explored all aspects of the chemical components found in the PDB archive. A presentation on *Using molecular structures from the PDB for a visual and exploratory learning experience in biochemistry* was part of the *Advances in Teaching* session.

Batsal Devkota, Monica Sekharan, and Chenghua Shao and the ChemLuminary Award. For more on the award from the ACS, see bit.ly/bsYNl2.

The North Jersey Younger Chemists Committee, led by RCSB PDB annotators Monica Sekharan (Chair), Bastal Devkota, and Chenghua Shao (Vice Chairs), was awarded the *ChemLuminary Award* for **Outstanding New Local Section**.

As part of the **BioCreative III Workshop on Critical Assessment of Information Extraction in Biology** (Sept. 13-15, Bethesda, MD), Andreas Prlić talked about the integration of open access literature with the RCSB PDB using BioLit and his work with the Distributed Annotation System protocol for exchanging biological data.

Director Helen Berman described the history of the PDB archive and the formation of the Worldwide Protein Data Bank organization at the Wolfram Data Summit (Sept. 9-10, Washington, DC).

Education Corner by Joan Kiely, Stony Brook University

Protein Challenge

Did you ever imagine insulin as a two-chain protein nestled in a knitted pancreas cozy? Draw a link between Willy Wonka and diabetes? See ribonuclease A as an aggressive toothed snake devouring stray RNA molecules? Students participating in the *Protein Challenge* see proteins just that way–as tangible things with form and function inextricably linked.

The Stony Brook University *Protein Challenge* is a competition for high school students. Working in teams, students research and build a model of a specific protein based on the structural data in the PDB. We select the *Protein Challenge* target protein from a *Molecule of the Month* feature at the RCSB PDB, and focus on a single protein file and associated paper, such as insulin in 2009 and epidermal growth factor receptor in 2010. Students are responsible for studying the published paper describing the structure, and for collecting sufficient background information to understand the function and importance of the protein. They then build a model of the protein using a foam-covered wire as the carbon backbone (Mini-Toobers from **www.3dmoleculardesigns.com**). Their creativity and understanding is demonstrated by the additions that they make to show significant side chains, ligands and other key features of the protein. The students also write a short essay explaining the function of the protein and how that is reflected in their model. They spend two months researching the protein and building their models. We evaluate the models for their accuracy and relevance to the function

JOAN KIELY *is the Director of the Biotechnology Teaching Centers (BTC) at Stony Brook University and the Principal Investigator of the Astellus Grant. In addition to overseeing the* Protein Challenge, *she teaches courses in microbiology for secondary school teachers, laboratory science curriculum development, and is developing a course for teachers on model systems in biology. She earned her Bachelor of Science degree in Microbiology from Michigan State University and a Master's Degree in Molecular Microbiology from Stony Brook University. After 18 years of biomedical research, she joined the faculty of CESAME in 2000.*

The Center for Science and Mathematics Education at Stony Brook University (CESAME) hosts the Protein Challenge *as part of an outreach program. CESAME's goal is to improve science education at the secondary and college levels. CESAME offers programs for high school students and teachers, undergraduates interested in research or teaching careers, graduate students, post-doctoral fellows, and faculty. The* Protein Challenge *is funded through a generous grant from Astellas Pharma US.*

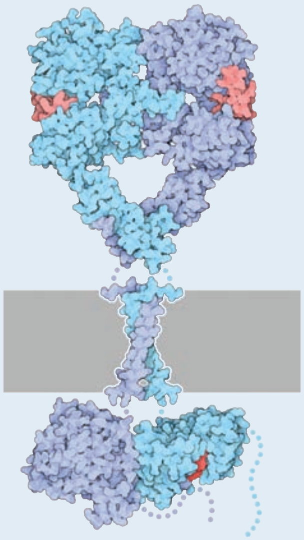
For more information, please see ***www.stonybrook.edu/cesame****.*

of the protein. On the day of the competition, the teams build another model of a shorter peptide and complete a short written exam to demonstrate that they have mastered the material.

The models are evaluated by teams of judges consisting of a graduate student in the Master of Arts in Science Teaching program (MAT) and a professional research scientist, either from Stony Brook University or from our sponsor. The judging teams are integral to meeting CESAME's goal of improving future science education by bringing together research scientists and future teachers. We award prizes for first, second and third place overall, best model and highest score on the exam. In addition we have a *People's Choice* category for which the students choose the winner.

This program is the result of a productive collaboration among the science education and research faculty at Stony Brook University, research scientists of Astellas Pharma US, and enthusiastic teachers from the participating school districts. The program was adapted from a program created by the Center for Biomolecular Modeling at The Milwaukee School of Engineering (**cbm.msoe.edu**).

After four years of the *Protein Challenge* we have learned many things. Foremost is that high school students are an inspiring group, capable of absorbing and synthesizing incredibly complex material. In addition, they will make insightful links when given the opportunity. For example, one team used pompoms to represent side chains; they put eyes on hydrophilic side chains because hydrogen bonds can be compared to looking at someone rather than holding hands as in a covalent bond. High school students are also eager and able to delve deeply into a topic, searching far and wide for information. Given the opportunity, they love to share what they have learned. During the *People's Choice* segment, you can hear students sharing detailed information and evaluating the models at a sophisticated level. A lunch is held to facilitate connections between research scientists and the students. This event has fostered many productive conversations about careers and opportunities in science. In the past, the winning teams have toured the OSI Pharmaceutical Research facility on Long Island. The lunch and tour interactions introduce students to new career options and give research scientists an opportunity to share their passions. In the first year, twenty teams participated; we are now running at full capacity with 36 teams, more than 400 students in four years.



Approximately 400 students from Long Island will compete in the next **Protein Challenge** on December 9, 2010. The event will look at lung cancer and anti-smoking campaigns while focusing on the epidermal growth factor receptor in complex with the chemotherapy agent Tarceva (PDB ID 1m17).

For information, see **www.stonybrook.edu/cesame/teachers/Competitions/ProteinModelingChallengeHome.html**

Epidermal Growth Factor was the Molecule of the Month *in June 2010 (doi: 10.2210/rcsb_pdb/mom_2010_6).*

Bringing research scientists together with MAT graduate students has been incredibly valuable for these students. These graduate students have all earned bachelor's degrees in a science discipline; in the MAT program they hone their teaching skills before moving on to teach secondary school science. This program gives them an opportunity to revisit their knowledge of basic chemistry, proteins and biology. The combination of building their own models and judging the models built by high school students reinforces the MAT students' understanding and confidence. The graduate students and research scientists work together as a team for approximately three hours. This close contact with a scientist leads to productive discussions about the process, the opportunities, and the joys of research. Our goal is that this exchange will enrich the teaching of high school science.

We have also learned that many high school science teachers are avid learners and anxious to bring the latest information into their classrooms. CESAME has close collaborative ties with area teachers though our outreach and continuing education programs. All the teachers involved in this program participated in workshops on molecular modeling either though CESAME at Stony Brook University or at the Milwaukee School of Engineering. Through these workshops, the teachers learn to use models and valuable online resources such as the RCSB PDB, Proteopedia and PubMed Central. During the competition, a faculty member from Stony Brook University leads a seminar for teachers. In the past, faculty have presented programs based on their work in cognition and cancer biology. This program is a practical way to gather teachers and scientists to share information.

When we started the Stony Brook University *Protein Challenge* we hoped to educate students and teachers about the cool stuff proteins do. We have been very pleased that this has succeeded to the extent that nine schools have gone on to develop extracurricular programs in protein modeling. We are most pleased to see the excitement and sharing that this program has fostered among high school students, graduate students, teachers, and scientists.

RCSB PDB PROTEIN DATA BANK NEWSLETTER

Web: www.pdb.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:

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San Diego Supercomputer Center and the Skaggs School of Pharmacy and Pharmaceutical Sciences
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The RCSB PDB is a member of the Worldwide Protein Data Bank (www.wwpdb.org)

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