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RCSB PDB PROTEIN DATA BANK NEWSLETTER

Contents

SNAPSHOT: JANUARY 1, 2010
62,388 released atomic coordinate entries

MOLECULE TYPE		EXPERIMENTAL TECHNIQUE	
57,728	proteins, peptides, and viruses	53,776	X-ray
2,087	nucleic acids	8,187	NMR
2,535	protein/nucleic acid complexes	266	electron microscopy
38	other	21	hybrid
		138	other

42,967 structure factor files
5,477 NMR restraint files

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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)

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

Message from the RCSB PDB

The recently-published 2009 Annual Report highlights recent accomplishments by the RCSB PDB. Milestones covered in this report include the release of the **PDB Archive Version 3.15** by the wwPDB, the implementation of the **MyPDB** service that notifies users when structures of interest are available, and the **redesign of the website**.

This 2009 edition is the RCSB PDB's tenth Annual Report. These bulletins were established to provide a yearly snapshot of RCSB PDB activities and the state of the PDB archive. It is distributed worldwide to researchers in biology, biochemistry, genetics, pharmacology, biophysics, and bioinformatics; computer scientists and software developers; and students and educators of all levels.

The Annual Report is available online from **www.pdb.org**. If you would like a printed copy, please send your postal address to **info@rcsb.org**.

Data Deposition and Processing

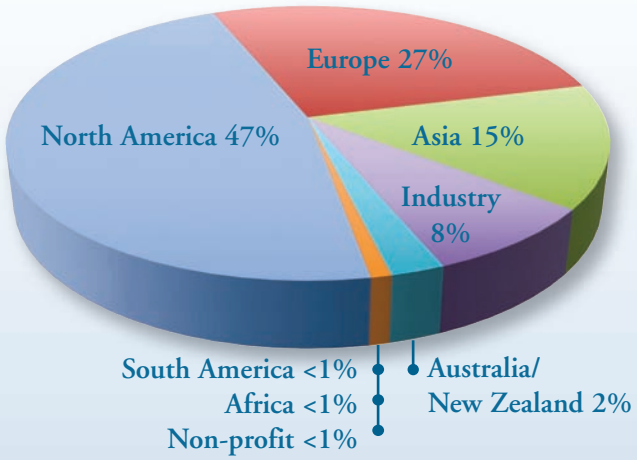
2009 Statistics

In 2009, 8298 experimentally-determined structures were deposited to the PDB archive, and then processed by wwPDB teams at the RCSB PDB, PDBe, and PDBj.

Of the structures deposited, 74.6% were deposited with a release status of HPUB; 22.8% were released as soon as annotation of the entry was complete; and 2.6% were held until a particular date. 92% of these entries were determined by X-ray crystallographic methods; 7.1% were determined by NMR methods.

7448 structures were released in the PDB archive in 2009.

Depositor Locations (8298 structures deposited in 2009)



Data Deposition Resources

Planning to deposit a structure in 2010? There are several resources available to help

The **Validation & Deposition Portal** contains links to software and documentation, including step-by-step deposition instructions specific for each experimental method:
deposit.rcsb.org

The **Deposition FAQ** answers Frequently Asked Questions about depositing structures and releasing the processed PDB entries:
deposit.rcsb.org/depoinfo/depofaq.html

The **Validation Server** checks the format consistency of coordinate files and produces validation reports that can highlight potential problems before a structure is deposited:
deposit.rcsb.org/validate/

For a depositor packet of printed materials, please send your postal address to **info@rcsb.org** with the subject line *first time depositor.*

Data Query, Reporting, and Access

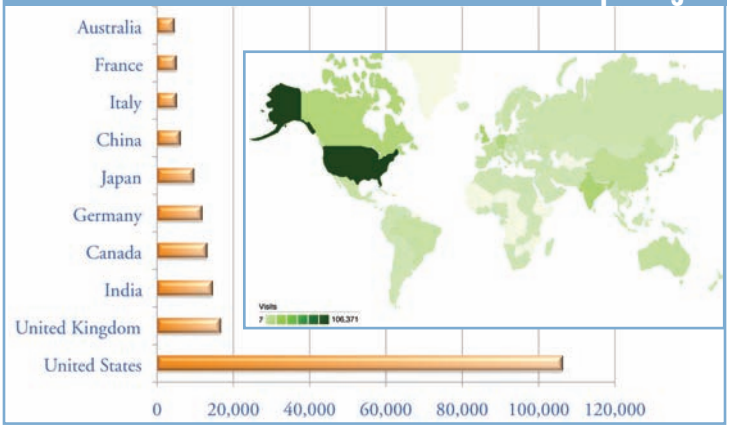
2009 Website Statistics

Month	Unique Visitors	Number of Visits	Bandwidth
JANUARY	160,293	355,392	634.85 GB
FEBRUARY	168,082	373,510	767.21 GB
MARCH	189,143	434,542	966.02 GB
APRIL	178,430	404,618	875.53 GB
MAY	164,084	380,493	835.61 GB
JUNE	145,958	356,857	1,079.61 GB
JULY	125,701	325,381	1,064.26 GB
AUGUST	119,287	315,040	914.56 GB
SEPTEMBER	163,204	403,770	980.24 GB
OCTOBER	195,573	471,869	1,144.92 GB
NOVEMBER	201,967	478,142	1,324.39 GB
DECEMBER	176,108	404,105	923.31 GB

2009 Visitors by City

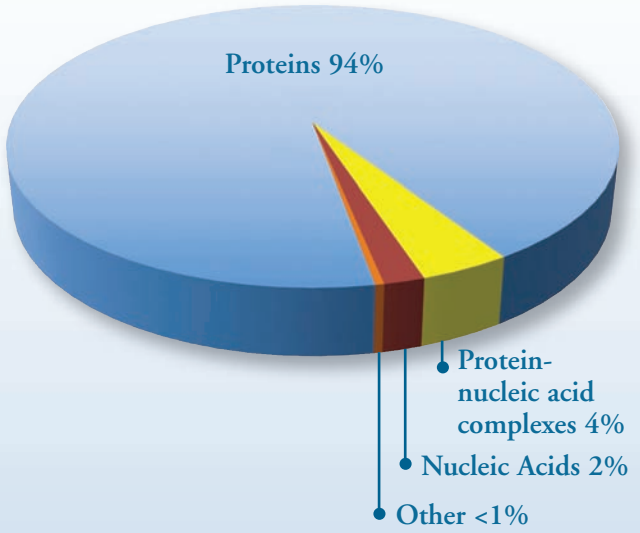
The RCSB PDB website had more than 4 million visits in 2009 by users in more than 15,000 cities. Image created using Google Analytics.

2009 Visitors to the Educational Resources of www.pdb.org



The RCSB PDB's Educational Resources, *including* Molecule of the Month *and* Looking at Structures, *had more than 300,000 visits by users in 144 countries in 2009. Top ten visiting countries are highlighted. Map image created using Google Analytics.*

2009 Molecule Type (7448 structures released in 2009)



New and Improved Web Services for Accessing PDB Data

Web Services can help software developers build tools that interact more effectively with PDB data. Instead of storing coordinate files and related data locally, Web Services let software tools interact with the RCSB PDB remotely.

The RCSB PDB supports RESTful services that exchange XML files in response to URL requests. RESTful search services return a list of IDs for Advanced Search and SMILES-based queries. RESTful fetch services return data when given IDs, including PDB entity descriptions, ligand information, third-party annotations for protein chains, and PDB to UniProtKB mappings. SOAP Web Services are also available.

Documentation for accessing these Web Services is available online. Improvements are being made based on community feedback. Please let us know if there are website options that you think should be offered as a web service at **info@rcsb.org**.

wwPDB FTP Advisory Notice

On November 24, 2009, a few changes were made to the wwPDB FTP directories. Updates were made to the RSYNC script and README files to prompt users to select which wwPDB server should be used (RCSB PDB, PDBe, PDBj).

Sequence cluster data was moved from the wwPDB FTP site to **ftp://resources.rcsb.org/sequence/clusters/**. This resource contains the results of the weekly clustering of protein chains in the PDB generated by BLASTClust. These clusters are used in the "remove similar sequences" feature on the RCSB PDB website. For more information on this feature, please see the README file and **www.rcsb.org/pdb/statistics/clusterStatistics.do**

Questions should be sent to the wwPDB at **info@wwpdb.org**.

New Website Features

A lot of new features have been added to **www.pdb.org**, including enhancements to browsing query results, generating tabular reports, and viewing large structures. Many of these features are described in this newsletter, but users should always check the WHAT'S NEW page for detailed descriptions of the latest updates.

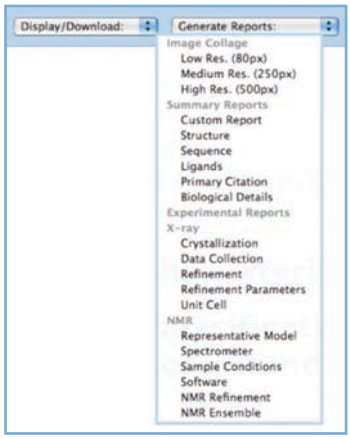
Latest Publications: Access All Articles in Each Update

Available from the left-hand menu, the new **Latest Publications** search returns the PubMed articles associated with PDB structures in the most recent update. It includes publications for newly released structures and for structures whose PubMed abstracts were added to our database in that update.

The results are presented in the Query Results Browser with the "Citations" tab highlighted by default. The other query results tabs are provided as well, so by clicking on the "Structure Hits" tab, all structures associated with these publications can be explored. Clicking on the first icon ( ) will download the citations in Medline format.

Improved Tabular Reports

For any search results, users can examine individual PDB entries or review the entire set of structures by creating reports that can be viewed online or downloaded. Recently, this reporting system has been enhanced with improved functionality and navigation, and now offers better support for very large result sets.



Prepared and customized reports can be generated for search results.

• Report Navigation

Reports can be generated for structures matching a query by selecting any of the prepared options available from the pulldown menu or by creating a new, customized report. Instead of presenting everything on a single page, reports are now available on multiple, customizable pages. By default, the first 15 records sorted by PDB ID are shown, with an option to list more records per page.

The entire table can be sorted by clicking on column headers. Column widths can be resized by dragging the line between two columns. Within the reports themselves, PDB IDs link to that entry's Structure Summary page, PubMed IDs to the abstract, and Ligand IDs to a Ligand Summary page.

• Exporting Reports

Tables can be exported in three formats: Excel 97-2003, Excel 2007 or newer, and or Comma Separated Value (CSV) format (recommended for extra large data sets that may surpass size limitations in Excel).

The Excel spreadsheets are formatted with customized column width, text wrapping, alignment, and hyperlinks on selected columns.

• Generating Large Reports

Reports can now be generated for extremely large sets of data. For example, a report displaying the X-ray Refinement Details (Rvalue, Rfree, and Resolution) can be made for all crystal structures in the PDB.

To generate this report, select **PDB Statistics** at top right of the RCSB PDB website, and click on the first link for **Summary Table of Released Entries.**

Selecting the number for X-RAY / Total will return the more than 53000 structures that match this query. From the navigation bar, click on **Generate Reports** and select **Experimental Reports/X-ray/ Refinement**. This report can be browsed, formatted, and downloaded as described above.

Other large reports, such as the summary reports for Biological Details and Sequence, can be easily generated for all structures in the PDB.

Improved Display of Large Structures

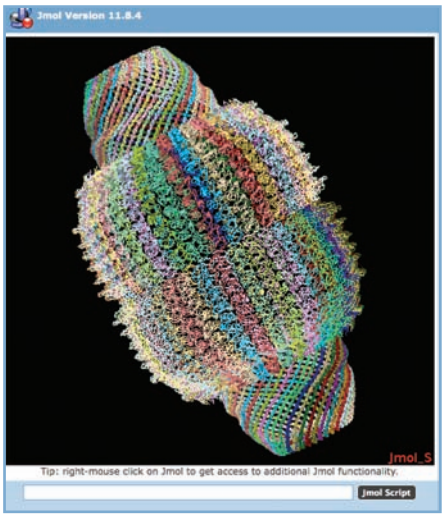
Images and Jmol[1] displays on the RCSB PDB website now show the complete biological assembly for all structures–even for proteins that are split across multiple PDB coordinate files.

A number of structures in the PDB archive are so large that the historical limitations of the PDB file format (maximum of 99999 atoms and 62 unique chains) require them to be split across multiple PDB coordinate files. Examples include extremely large ribosome complexes (e.g., 1gix, 1giy), and structures that contain a very large number of atoms or chains, such as the vault protein (e.g., 2zuo, 2zva, 2zv5).

These structures are identified on Structure Summary pages in the new "Split Entry" box, which lists and links the PDB IDs of all entries that make up the composite structure. A link is provided to easily download all of the related coordinate files.

Images on the Structure Summary page now illustrate the full composite structure, rather than what is found in each individual PDB coordinate file. The image on the Structure Summary page for 1gix, for example, shows the full ribosome structure composed of entries 1gix and 1giy. For all Structure Summary images, the forward and backward buttons can be used to toggle between the asymmetric unit and the biological assembly (or multiple biological assemblies, if applicable) for the full structure.

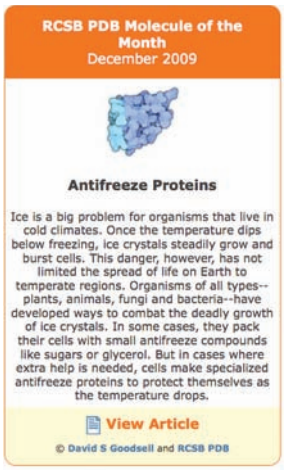
The biological assembly and asymmetric unit of the composite structure can be launched in Jmol when viewing the corresponding static image. The display of such large structures in Jmol is possible by loading PDB files limited to CA and P atoms, and by using the Jmol load files command.



The vault structure represented by entries 2zuo, 2zva, 2zv5 can now be viewed in a single Jmol viewer at the RCSB PDB.

H. Tanaka, K. Kato, E. Yamashita, T. Sumizawa, Y. Zhou, M. Yao, K. Iwasaki, M. Yoshimura & T. Tsukihara (2009) The structure of rat liver vault at 3.5 Ångstrom resolution. Science 323*: 384-388.*

Use Widgets to Embed RCSB PDB Features on Your Website



These widgets link directly to the RCSB PDB website so users don't have to download any files. The Molecule of the Month *widget can be used to link to a particular feature, or it can be set to be automatically updated when new features are published.*

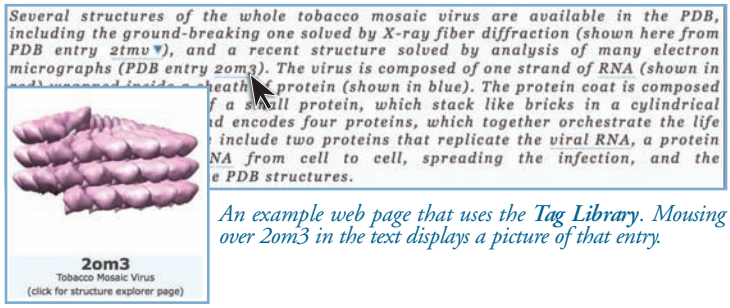
Molecule of the Month images and text, static images and interactive views for any PDB structure, and RCSB PDB searches based on ID and keyword can be embedded into any website using the RCSB PDB's web widgets. These small bits of code can be customized to display and link to RCSB PDB features.

• The ***RCSB PDB Molecule of the Month* widget** embeds an image from the feature and links to the entire article. The widget can be customized to specify width, colors, amount of text shown, and molecule.

• The **Tag Library** can be used to embed an image that links to the corresponding Structure Summary page; provide a menu of links to a particular entry's Jmol view, Structure Summary Page, and PDB file; and provide a link that performs a current keyword query.

• The **Image Library** widget embeds an image of a structure based on PDB ID.

These widgets bring RCSB PDB functionality to any resource. For more information and other widgets, see the Widgets page linked from the Tools section of the RCSB PDB's left menu.



An example web page that uses the ***Tag Library****. Mousing over 2om3 in the text displays a picture of that entry.*

Improved Advanced Search Interface and Help

A new Advanced Search interface helps users build complex queries in a more intuitive manner. Search criteria are more clearly defined, and the overall design makes it easy to add and remove search parameters.

Advanced Search is a tool that can be used to combine a variety of simple searches into a single query, such as: *Which proteins have ligands (but not any nucleic acids)? What protein-serine/threonine kinases were released in 2008? How many structures with resolution less than 2.0 Å contain a given sequence motif?*

Advanced Search has been enhanced with a new intuitive help system that will eventually replace the current robohelp system. The Advanced Search help system displays help, query definitions, and examples based upon what is shown on the screen. For example, selecting ? at the first Advanced Search page will return an overview of the query feature, while selecting ? when looking at the window for Secondary Structure Content returns context-related search criteria and examples. By default, the new help system opens in a shadow box interface, but can also be viewed in a separate window by clicking on the pop-up link.

Outreach and Education

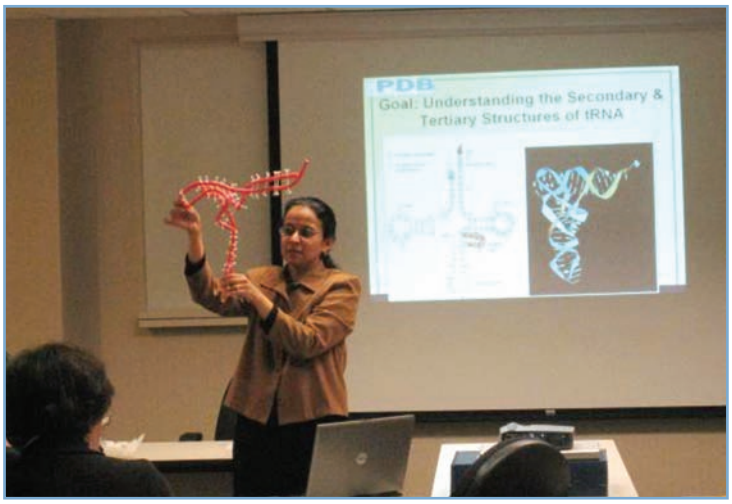
Poster Prize Awarded at ECM

Yonca Yuzugullu

Yonca Yuzugullu was awarded the **RCSB PDB Poster Prize** at the **25th European Crystallographic Meeting** (August 16-21, 2009; Istanbul, Turkey) for Crystallization of bifunctional catalase-phenol oxidase (CATPO) from *Scytalidium thermophilum*. Yonca Yuzugullu, Chi Trinh, Arwen R. Pearson, Mark A. Smith, Simon Phillips, Ufuk Bakir, Michael J. McPherson, Zumrut B. Ogel (Middle East Technical University, Turkey).

Many thanks to Elspeth Garman (University of Oxford) and Joel Sussman (Weizmann Institute of Science) for judging the posters, and to Andreas Roodt (University of the Free State, South Africa) for organizing the judging.

Recent and Upcoming Meetings



Science teachers at the NJSC learned how to build tRNA–from a cloverleaf representation into a 3D paper model–through a presentation by Shuchismita Dutta.

At the **New Jersey Science Convention** (NJSC; October 13-14; 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 tRNA structures out of paper during a presentation by Shuchismita Dutta.

From December 5-9, the RCSB PDB exhibited at the **49th Annual Meeting of the American Society for Cell Biology** in San Diego, CA alongside the PSI Structural Genomics Knowledgebase (PSI SGKB). David Goodsell, author of the *Molecule of the Month*, discussed *Visual Representation from Atoms to Cells: New Work from the Machinery of Life* as part of a session on Exploring Cell Biology at the Frontier of 3D Visualization.

John Westbrook chaired a session on Ligands in the PDB at the **eCheminfo Community of Practice Meeting on Advances in Drug Discovery and Development** (October 13-16; Philadelphia, PA). The session, a continuation of a session chaired by Marc Nicklaus (National Institutes of Health) at the 2008 eCheminfo meeting, explored issues related to interpreting ligand structural data in the PDB.

Presentations included *Ligand Pocket Detection in Biological Assemblies* (Howard Feldman, Chemical Computing Group), *Conformer Generation: Finding and Learning from Failures* (Paul Hawkins, OpenEye Scientific Software), *The PDB and Antibiotic Peptide Sequence-like Compounds* (Kim Henrick, PDBe), *Thoughts about Ligand-Structure Validation* (Gerard J. Kleywegt, PDBe), *electronic Ligand Builder and Optimisation Workbench (eLBOW): A tool for Ligand Coordinate and Restraint Generation* (Nigel W. Moriarty, Lawrence Berkeley National Laboratory), *Ligand Energies Calculated Quantum-Chemically in Vacuum and Solvent Model* (Marc Nicklaus), *Iridium: Marginally Less Bad than the Rest* (Gregory L Warren, OpenEye Scientific Software, Inc.), *Enabling the World of Internet Based Chemistry Through ChemSpider* (Valery Tkachenko, Royal Society of Chemistry), and *Mitotic Kinesin Eg5 Inhibitors Generation By Computational MED-Portion Based Drug Design at PDB Scale* (François Delfaud, MEDIT).

At Cold Spring Harbor Laboratory's course **X-Ray Methods In Structural Biology** (October 12-27), John Westbrook presented PDB Tools for Depositors.

Helen Berman described the process of *Annotation of Carbohydrates* in the PDB at the NIH's **Workshop on Leveraging Glycan Array Screens with Biological, Computational and Structural Data** (October 22-23, Bethesda, MD).

Phil Bourne presented *The Changing Landscape of Scholarly Communication as it Relates to the Biosciences* at the 19th Keck Center Annual Research Conference on **Computation in Biology: from Gene to Neuron** (October 29-30, Rice University) and *The Evolution of Protein Structure and Function as Studied through Structural Bioinformatics* at the 18th Annual **Buffalo-Hamilton-Toronto Symposium** (November 6, McMaster University)

The San Diego Section of the American Chemical Society (ACS) celebrated National Chemistry Week by holding **CHEM EXPO** in Balboa Park (November 1). At the RCSB PDB booth, middle and high school students, plus parents and teachers, learned about drugs and proteins using a variety of materials and displays.

*Peter Rose demonstrated the resources of the RCSB PDB to visitors to the ACS **CHEM EXPO**, held in Biloba Park, San Diego.*

Future meetings include the **Keystone Symposia Frontiers of NMR in Biology** (January 8-13, 2010; Breckenridge, CO) the **Biophysical Society Annual Meeting** (February 20-24; San Francisco), and the **National Science Teacher Association's Annual Meeting** (March 18-21; Philadelphia, PA). 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**.

Education Corner by IJsbrand M. Kramer, Ph.D., University of Bordeaux1

A Search for the Best Methods to Illustrate Complex Information

Structure-based function analysis of cellular components has expanded rapidly over recent years and has consequently led to the development of a new semiotic system for teaching.[2] The infographic approach has shifted from a schematic towards a more realistic representation of cellular components. The radical difference in conceptual artwork of cell and molecular biology (and biochemistry) in current course books compared to those of only 10 years ago exemplifies this change.

Realistic illustrations of "invisible" subcellular objects closely resemble experimentally-derived structures of cellular components and are characterized by a low level of styling and simplification.[3; 4] In contrast to the representation of macroscopic objects, where realistic images are generally easy to understand because they bear direct visual references to everyday life objects, realistic images of microscopic objects are necessarily difficult to understand because they lack visual reference–on top of that, they tend to be complex! Microscopic objects cannot be observed by the naked eye. Worse, the raw experimental data obtained from crystallographic X-ray diffraction or NMR studies have proven incomprehensible to the non-expert brain. Digesting these experimental results requires computer-aided image processing and this implies that the depiction of microscopic objects is necessary representational and thus "abstract". With reference to the cognitive load theory, cell and molecular biology images always carry a high intrinsic cognitive load.[5; 6] Independent of the type of representation chosen, being realistic or schematic, these images are difficult because they require a thorough understanding of numerous iconic (object represents a molecule) and scientific codes (object represents a membrane receptor involved in a signaling cascade) in order to be meaningful.[7]

In cell biology teaching, I discern a number of forces driving towards the adoption of realistic images. Firstly, structural analysis provides a much more meaningful understanding of the functioning of cellular components, and in particular of proteins.[8; 9] Secondly, many cellular processes seem to occur in multi-protein complexes (comprising scaffold, adaptor and effector proteins), kept together by domain-specific interactions. While attempting to represent schematically the different domains and how they form protein assemblies, one quickly asks the question; what does it really look like? Thirdly, students have to be prepared for the post-genomic era, characterized by an explosion of genes, gene products and structural analyses. Ideally, they should be confronted with the new infographic approach at an early stage in order to prevent a very steep learning curve at the end of their studies. Finally, many teachers have a natural tendency towards the inclusion of state-of-the-art molecular representations because they reflect better their level of understanding. This tendency is encouraged by the ample supply of state-of-the-art scientific illustrations in science (review) journals, by the availability of web-based tools for macromolecular visualization and, last but not least, by easy access to the 3D coordinates of macromolecules via the PDB.

Not all university teachers follow this path. Some strongly oppose realistic images and advocate to keep things simple for introductory courses because images only have to convey the "basic principles and concepts" of cell biology. Others are reticent simply because they themselves fail to provide meaning to the novel infographic approach or lack the molecular-graphic and multimedia skills necessary to embark on the transformation process. All the above arguments are valid from a teachers' point of view, but teachers are experts, and experts tend to forget how the unprepared mind functions (or how their unprepared mind functioned)[10]. What really matters is to find out what our learners read in the images we provide.

I therefore have set out a series of tests, in collaboration with Hassen-Reda Dahmani and Patricia Schneeberger (University Victor Segalen Bordeaux 2), in which students attending an introductory cell biology course at the University of Bordeaux 1 (first year Life and Environmental Sciences) were confronted with images that represented the same cellular component but with different infographic approaches (see Figure 1 as one example)[4]. In order to prevent conditioned reflexes, none of these images strongly resembled the ones used in the accompanying teaching documents (**www.cellbiol.net/cbe/multimedia.php**). What we learned was that our first year students can handle complex realistic images and that the apparent complexity does not deter them from investigating their meaning.[4]

IJSBRAND KRAMER *(i.kramer@iecb.u-bordeaux.fr) is a professor at the University of Bordeaux, working in the European Institute of Chemistry and Biology (IECB). He holds a bachelors and masters degree in BioMedicine from the University of Utrecht, The Netherlands, with a one year research-excursion in the Department of Cell Biology at the University of Liverpool, UK. He did his Ph.D. at the University of Amsterdam, in the Central Laboratory of Blood transfusion services (Stichting Sanquin) and worked as a post-doctoral fellow at the Hubrecht Laboratory in Utrecht and at the University of Washington in Seattle. He then took a lecturer position at the Department of Pharmacology at University College London, where, together with Bastien Gomperts and Peter Tatham from the same University, he wrote the much renowned textbook on Signal Transduction. The second edition was recently published by Academic Press/Elsevier. More information about his teaching and research activities can be found at* **www.cellbiol.net**.

Using jigsaw puzzles allows students some time to contemplate the structure of the c-Abl tyrosine protein kinase bound to one of the inhibitors used in the treatment of chronic myelogeneous leukemia (CML).

We like to stress, however, that when teachers adopt a realistic iconographic approach, the images should naturally be accompanied by coherent explanatory text, relevant knowledge evaluation, and an engaging environment that encourages the learner to develop mental representations of the subjects in question.[11] Perhaps one of the most challenging aspects of current cell biology education is designing course instructions that without denying the complexity of cell functioning, allow students to access the complexity in a meaningful way. An approach that allows them to develop relevant schemas (mental images, models) with which they are able to construct, over the years, an operational understanding of the cell needs to be used.[5; 6; 12-14] Together with Graham Johnson (The Scripps Research Institute) and Lena Tibell (University of Linkoping), and thanks to funding by the National Science Foundation, this research project is now being pursued in a much broader teaching environment.

These reflections about teaching, and the ensuing pedagogical study, have been instigated in part by the desire to construct learning documents (web-based multimedia resources as well as books) that could accompany the learner throughout the learning path, starting at the university and beyond–life-long learning. Through teaching both first and third year students, I realized the convenience of adopting a universal (realistic) infographic approach; it allows me to smoothly integrate first year cell biology course material with the third year signal transduction teaching. I also discovered that the approach to conceptual artwork described above has the important advantage of being more amenable to an accompanying hands-on molecular modeling practical (biocomputing practical); there is less discrepancy between what students obtain on the computer screen, what they may encounter in the literature, and what they see in their teaching documents. Linking lecture content with hands-on molecular modeling, seeing and doing, enhances students' understanding of the nanoscale world.[15] The PDB has therefore become a key source for my educational endeavor.

Students are not my only concern: After 20 years of teaching I also learned that pedagogical (what to teach) and didactical (how to teach it) innovations provide me with the necessary "reward" to sustain teaching activities (in particular in moments where university management, teachers and students alike seem to have forgotten the real purpose of education). The pedagogical activities developed by the RCSB PDB, in particular, the work by David Goodsell, continue to be an inspiring and comforting source of information, as are the many other outstanding annotated databases in life sciences.

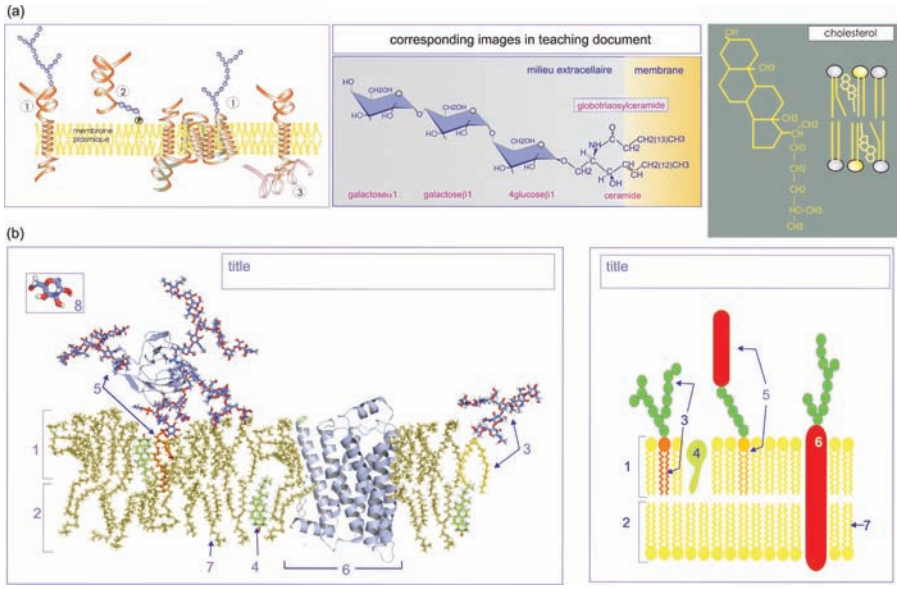


FIGURE 1. *Realistic versus schematic representation of the plasma membrane. (a) Course images of the plasma membrane; three relevant images from the teaching document are shown. (b) Test images of the plasma membrane: realistic representation (left) and schematic representation (right). The membrane components in the realistic representation are all based on experimentally derived structures. The phospholipid bilayer coordinates were obtained from equilibrated structures after molecular dynamics simulation (N. Taib), and the coordinates of the Thy1-glycosylated peripheral membrane protein were provided by M. Wormald. The structure of the β2-adrenergic receptor (PDB ID: 2rh1)[16] and of cholesterol (PDB ID: 1ssj)[17] were obtained from the PDB. The glycerol-glycolipid is a compilation of diacylglycerol combined with one of the sugar chains of Thy1 (an Adobe Photoshop cut-and-paste preparation). The schematic representation was found on the web and modified for our purposes. Students had to provide a title [cell membrane, lipid bilayer with (glyco)proteins] and label the numbered components: 1) membrane outer leaflet; 2) membrane inner leaflet; 3) glycerol-glycolipid; 4) cholesterol; 5) glycosylated peripheral-membrane protein (Thy1); 6) transmembrane protein (β2-adrenergic receptor); 7) phospholipids; and 8) sugar or hexose (only in realistic representation). In the schematic representation test, students had to decipher the iconic code for the green (sugar or hexose) and yellow (phospholipid headgroups) spheres. Finally, they were asked to provide a stick representation of a phospholipid. Figure and caption reprinted from Dahmani et al.[4] with permission.*

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

Rutgers, The State University of New Jersey
Department of Chemistry and
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

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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.pdb.org.

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www.pdb.org • info@rcsb.org
Department of Chemistry and Chemical Biology
Rutgers, The State University of New Jersey
610 Taylor Road
Piscataway, NJ 08854-8087
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