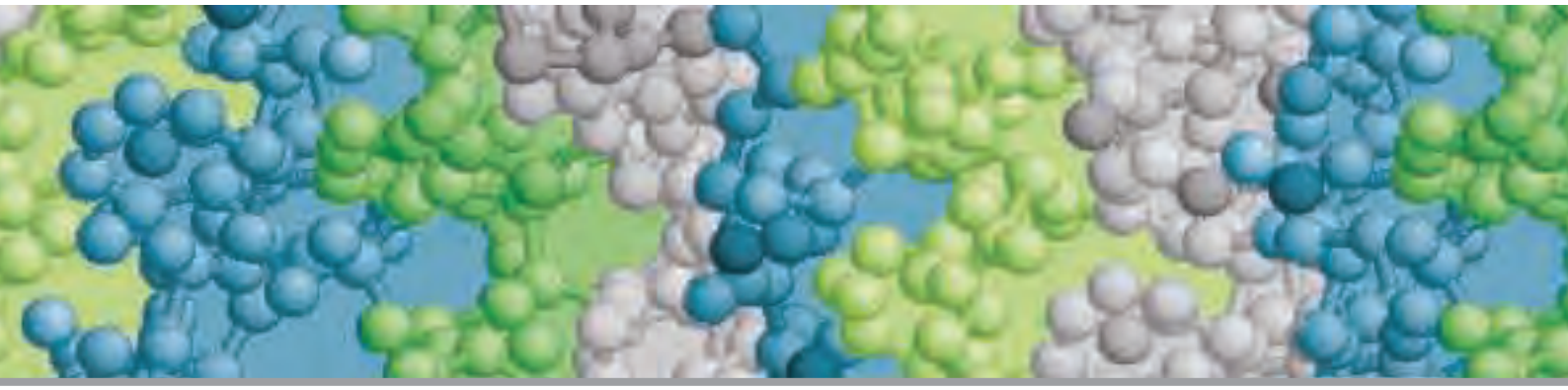
PDBj
Protein Data Bank Japan

http://www.pdbj.org/

News Letter Vol. 10, No. 1

November 2008



PDBj is maintained at the Protein Research Institute, Osaka University, and supported by Japan Science and Technology Agency.

News

The 5th wwPDBAC meeting

PDBj manages the PDB database and develops several services and software tools as a member of the wwPDB (worldwide PDB), which was founded in 2003, collaborating with RCSB-PDB in USA and PDBe-EBI in EU.
On September 29, 2008, the 5th wwPDBAC (wwPDB Advisory Committee) meeting was held at EBI, Hinxton, UK, by PDBe-EBI. The current situation and the future issues were presented and discussed by the participants: The members of the wwPDB, Prof. Helen M. Berman (RCSB-PDB), Dr. Kim Henrick (PDBe-EBI), Prof. Haruki Nakamura (PDBj), Prof. John L. Markley (BMRB), the AC members who are specialists in several fields of the structural biology: X-ray crystallography, NMR, and Bioinformatics, Dr. Stephen K. Burley (Chair), Prof. Wayne A. Hendrickson, Dr. Neil Isaacs, Prof. Rob Kaptein, Dr. Gerard J. Kleywegt, Prof. Kei Yura, and Prof. Soichi Wakatsuki. In addition, as the representatives of the International Societies of Crystallography, NMR and electron microscopy, Prof. Edward N. Baker (IUCr), Dr. Andrew Byrd (ICMRBS), and Prof. Marin van Heel (Macromolecular EM) attended the meeting. This time, the director of EMBL-EBI, Dr. Janet Thornton, and Rebecca Aarons from Wellcome Trust also attended the meeting.

The participants of the wwPDBAC meeting held on Sept. 29, 2008 at EBI, Hinxton, UK.

The members of the wwPDB: From left to right, J. L. Markley, K. Henrick, H. M. Berman, and H. Nakamura.

At the beginning of the wwPDBAC, it was announced by Dr. Janet Thornton, the director of EMBL-EBI that Dr. Kim Henrick, the head of PDBe, will leave his position in June, 2009, and all the wwPDB and wwPDBAC members appreciated his great efforts and contributions to the wwPDB. It was also announced that Dr. Gerard Kleywegt will become the head of the PDBe from June, 2009.

In this wwPDBAC meeting, the continuous effort to increase the data quality was appreciated, and a new policy that the NMR chemical shifts deposition should be mandatory with the condition of the future approval by the NMR society was introduced as one of the policies clarified by the NMR Task Force. The PDB new format, version 3.2, is being established so as to create a more uniform archive, and all files in the archive will be brought up to the new version 3.2 in 2009. Among several features of the new standard, the "SPLIT" record will be newly introduced for very large molecular structures to indicate several PDB entries. In addition, the new activity, in which all the wwPDB members are involved, was reported to develop a common deposition and annotation tool in 2009-2011 with delivery by 2012, because this issue was selected as the most important project by participants of the 2007 wwPDB Retreat held at Princeton.

Finally, the funding resource of the wwPDB activity was discussed, because there is no direct funding at the moment. New ideas to ask the international organizations were argued for the near future plan to establish the financial basis of the wwPDB.

The next 6th wwPDBAC meeting will be held in autumn of 2009, at Osaka, Japan, by PDBj.

The 8th Annual Meeting of the Protein Science Society of Japan

The 8th Annual Meeting of the Protein Science society of Japan was held from May 10th to 12th, 2008 at the Tower Hall Funabori in Tokyo. We introduced our activities and provided suggestions for PDB deposition.

Ichou Festival

The annual university festival, known as Ichousai, was held at Osaka University on May 2nd and 3rd. The laboratories and institutes were opened to the public, including high school students. We introduced the eProtS database, which is described further in this issue.

IUCr2008 in Osaka

The XXI Congress of the International Union of Crystallography Congress and General Assembly was held at the Osaka International Convention Center from 23rd to 31st August. The we exhibited a booth on 24th - 27th and introduced our activities. We appreciate all people who contributed to our successful exhibitions.

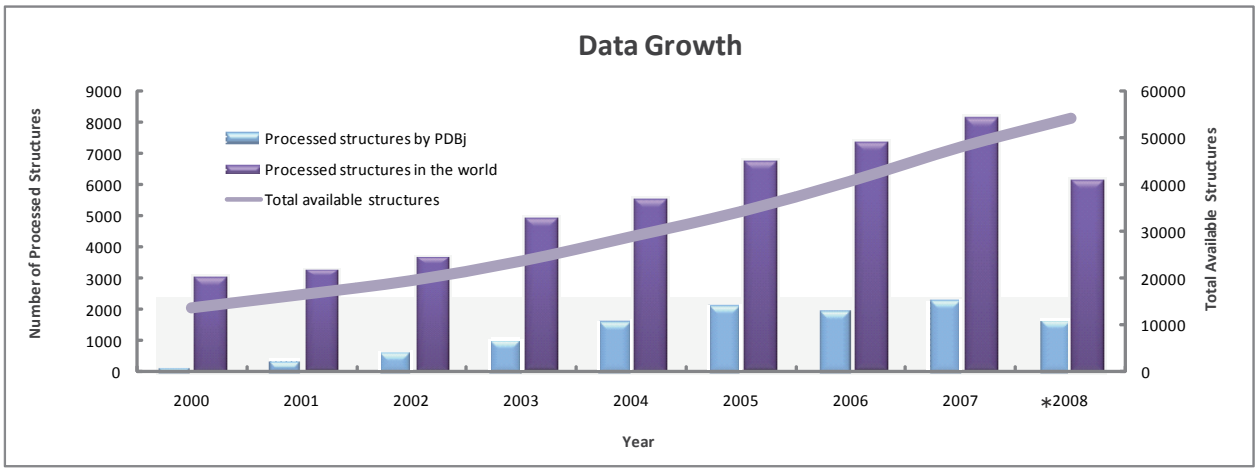
Snapshots of the 8th PSSJ.

Snapshot of Ichou Festival.

Snapshots of IUCr2008.

Statistics

The statistics data is available at the wwPDB page (http://www.wwpdb.org/stats.html).



* Last updated : November 12, 2008

Services

*Pro*Mode: Database for normal mode analysis of proteins

Although normal mode analysis (NMA) of proteins requires much less computational time than molecular dynamics, it still requires significant time to minimize conformational energies for typical PDB entries. In addition, although NMA can calculate several kinds of physical properties, such as fluctuations of atoms and dihedral angles both for a time average over all modes and for individual normal modes, the outputs of the results are too huge to provide on the WEB. Accordingly, the results provided in *Pro*Mode are limited. However, some researchers may be interested in the results not provided in the database for a specific protein. Therefore, we have begun to provide the following services.

(1) We have developed a stand-alone application with a user-friendly graphical user interface to enable the NMA calculation of a protein molecule by a user. Since our application uses intermediate results provided in the NMA calculation for *Pro*Mode, such as the data on the energy-minimized conformation and the eigenvalues and eigenvectors corresponding to all normal modes for a given protein, NMA can be performed for any specified mode in less than a quarter of an hour on both Microsoft Windows and Linux. The program generates not only the time-average data of the fluctuations of atoms and dihedral angles but also data required to display a three-dimensional (3D) animation of the vibrational motion of a protein molecule and to display the 3D atomic displacement vectors for the specified mode. The results thus obtained may be subsequently used in a spreadsheet application such as Microsoft Excel to prepare a data chart (Fig. 1). This application can provide more elaborate NMA data on a protein than *Pro*Mode.

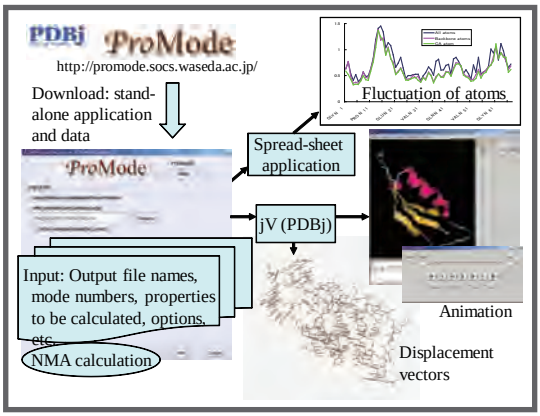


Fig. 1. Flow diagram of the normal mode analysis using the stand-alone application and data downloaded from ProMode.

(2) *Pro*Mode displays an animation of a vibrating protein molecule. The data for the animation can be downloaded. A user can operate the animation on the users local computer with the jV viewer downloaded from PDBj.

The above application and data can be downloaded from the relevant page of a protein of interest.

SeSAW: functional annotation by Sequence-derived Structure Alignment Weights

SeSAW is a functional annotation server that identifies conserved sequence and structural motifs in query proteins. The query can be an experimentally determined structure or a structural model. The latter case allows putative functional sites to be identified directly from sequence via an intermediate structural model. Similar to Structure Navigator, SeSAW first identifies all PDBj entries that are structurally related to the query. The functional significance of each structural match (template) is then assessed by profile-profile sequence comparisons anchored by the structure-based sequence alignments. Functional sites, when available, are then mapped from the templates onto the query-template alignments. A list of the templates, sorted by a scores for estimating functional similarity is returned, with links to both the annotated alignments (via the Jalview alignment editor) and the 3D structural superpositions (via jV)

SeSAW uses a target function that integrates sequence and structural information at the residue level in order to assess the functional significance of structurally aligned residues pairs [1]. The target function was optimized for distinguishing protein pairs belonging to the same family or superfamily from those that share the same fold but belong to different families or superfamilies. The method was originally used to functionally annotate all hypothetical proteins solved in the Protein 3000 structural genomics project in Japan [1, 2]. We have since discovered that the same approach can be used to identify functional sites in structures built by threading or homology modeling [3].

To use SeSAW, simply type in a PDB ID or upload a PDB-formatted file. If your query is a homology or threading model, it is important to provide SeSAW with the template PDB and chain ID, since this information will

be used to identify structurally related entries. You have the option of selecting email notification or have the results sent directly to your web browser as they are completed. Since all queries are computed in real time, and some queries can take over an hour to finish, email notification is the default behavior. Results will be stored on our server for two weeks.

The main results page is illustrated in Figure 1. In figure 1A, the template names appear at the leftmost column, and are linked to their summary page at PDBj. The SeSAW score and sequence identity are listed, along with the CATH or SCOP domain names, if available. In the alignment column, a link to the annotated alignment is given. In Figure 1B, the alignment, displayed using the Jalview alignment editor, is shown. The alignment indicates the residue positions of known functional sites (if available), the secondary structure of the template, and the residue-based SeSAW score. If functional annotations exist for the template an "*f* " appears next to the alignment link. In the last column, a link to the query-template structural superposition is given. The alignments and superpositions are computed using ASH, and displayed using jV. As shown in Figure 1C, in the jV applet window, stick representations of high-scoring aligned residue pairs between the query and the template can be turned on and off, enabling clusters of structurally or functionally important residues to be identified.

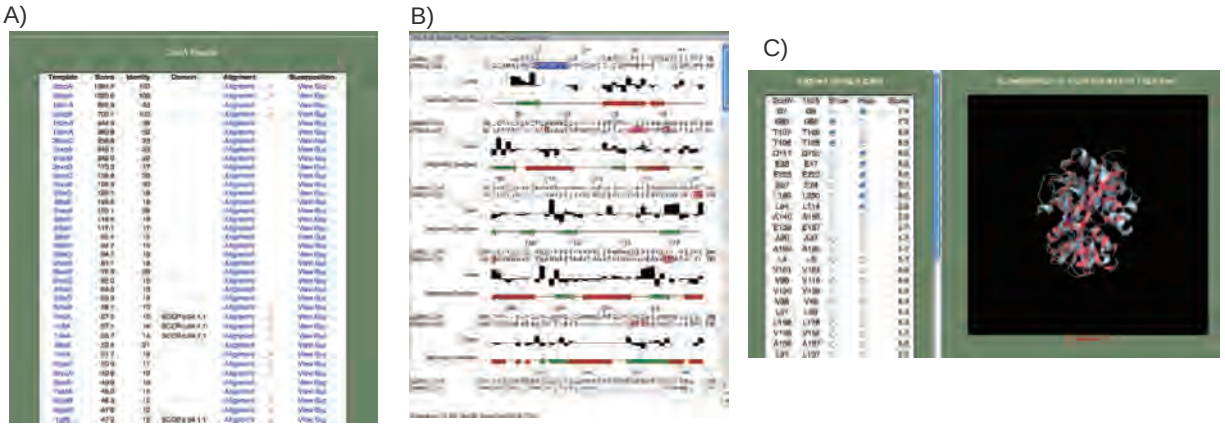


Figure 1. The figure shows the SeSAW results for the structural genomics target 2czl, chain A. A) The main results page lists templates in order of their predicted functional similarity to the query. In this case, most of the highest-scoring templates are themselves SG targets; however, a cluster of templates just below this group all have the common amino acid binding function. B) The alignment between 2czlA and 1ii5A, rendered by the Jalview alignment editor, is shown. The residue-based score is indicated by a bar-graph; some of the high-scoring residue pairs correspond to a conserved glutamate binding site (pink boxes). C) The structural superposition between 2czlA and 1ii5A is shown with residues lining the glutamate binding site selected and shown in stick representation.

References

1. Standley DM, Toh H, Nakamura H. Functional annotation by sequence-weighted structure alignments: statistical analysis and case studies from the Protein 3000 structural genomics project in Japan, Proteins 2008;72:1333-1351.

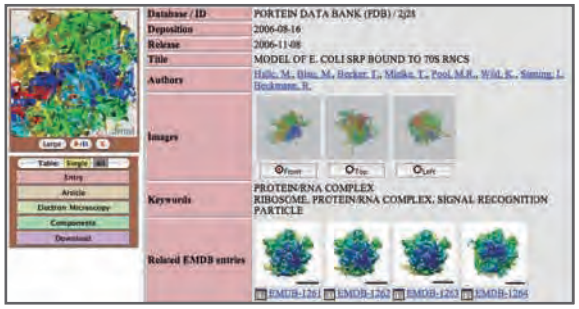
2. Standley DM, Nakamura H. From structures to functions: annotation by structural bioinformatics, Tanpakushitsu Kakusan Koso 2008;53:638-644.

3. Standley DM, Kinjo AR, Lis M, van der Giezen M, Nakamura H. Structure-based functional annotation of protein sequences guided by comparative models. Optimization and Systems Biology 2008;395-403.

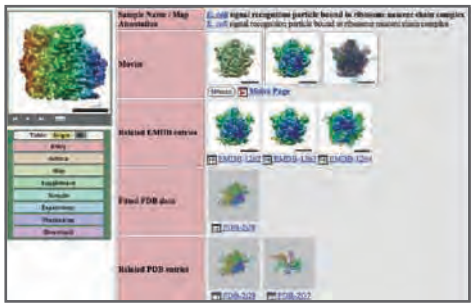
EM Navigator

EM Navigator started last spring, and has since been growing. EM Navigator is a web service for searching and browsing structural data obtained by 3D electron microscopy (3D-EM), and started as a data browser for the EM databank (EMDB) established by EBI in Europe. EMDB and PDB are similar but distinct databanks. The principle data of PDB and EMDB are atomic coordinates obtained by methods such as X-ray crystallography and 3D density maps obtained by 3D-EM, respectively. Additional information about the samples and experimental methods are deposited on both databanks as well. Which databank are the atomic-coordinates obtained by 3D-EM to be deposited? The answer is PDB. Structural data from 3D-EM are deposited on EMDB and/or PDB, depending on their data types. As hybrid-analysis methods have been gaining attention recently, repositories of such data are also hybrid and represent a rather complicated situation.

On the new EM Navigator, you can search and browse 3D-EM data in the PDB using the same interface as used to search the EMDB. On the detail pages for PDB entries, molecular viewers (jV and Jmol) are embedded to facilitate browsing the 3D structures interactively. Also, hyperlinks for related EMDB/PDB entries are shown with snapshot images to clear the relationship among the entries. To make it easy to search, browse and, enjoy 3D-EM data, we will continue to develop EM Navigator.



Details page of PDB-2j28.



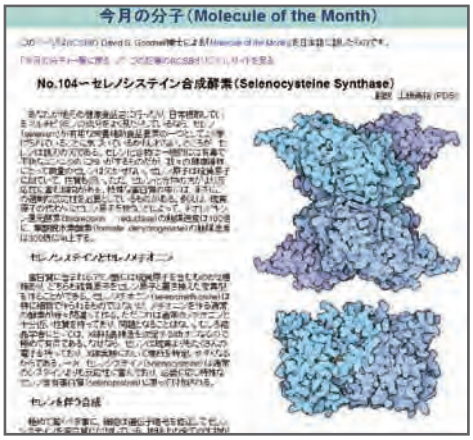
Details page of EMDB-1261.

Japanese “Molecule of the Month: MOM” site started

In April 2008, the number of monthly articles of "Molecule of the Month: MOM", which are produced by Dr. David S. Goodsell and appear at the RCSB-PDB Web pages, reached 100. Since then, we began releasing translations parallel to RCSB-PDB (http:// eprots.pdbj.org/mom/mom_j.html).

These articles present short accounts on selected molecules from the Protein Data Bank. Each installment includes an introduction to the structure and function of the molecule, a discussion of the relevance of the molecule to human health and welfare, and suggestions for how visitors might view these structures and access further details, including an interactive 3D viewer site using the Jmol applet.

It also can promote knowledge of structure biology by relating it to familiar events. As with eProtS (Encyclopedia of Protein Structure), this expands our activities to a more general audience. In the future, we are going to enrich eProtS by adding references to MOM and by including MOM entries in the eProtS search target.



An example of Japanese MOM page.

Contacting

PDBj
Research Center for Structural and Functional Proteomics,
Institute for Protein Research (IPR), Osaka University
3-2 Yamadaoka, Suita, Osaka 565-0871, Japan
TEL (PDBj office): +81-(0)6-6879-4311
TEL (PDBj deposition office): +81-(0)6-6879-8638
Director
Prof. Haruki Nakamura (IPR, Osaka University)