PDBj
Protein Data Bank Japan

http://www.pdbj.org/

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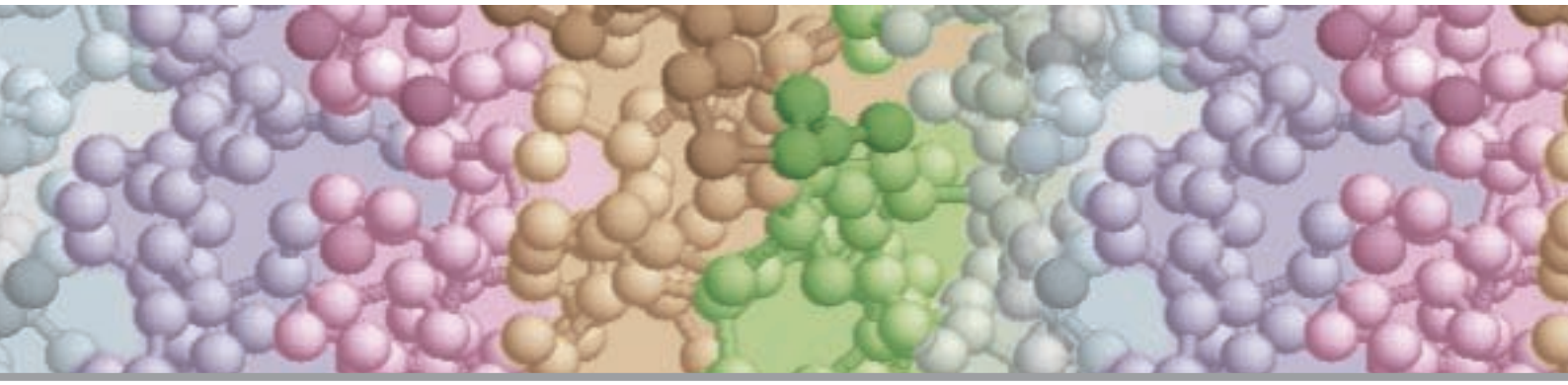


PDBj is maintained at the Protein Research Institute, Osaka University, and supported by Japan Science and Technology Agency.

News

New PDBj homepage

We have had a major re-design and added a Chinese page.

Center: English page, Left: Chinese page, Right: Japanese page.

PDBj and wwPDB

PDBj manages the PDB database and develops several services and software tools as a member of the wwPDB, which was founded in 2001, collaborating with RCSB in the USA and EBI in the EU.

Following the advice of the wwPDB Advisory Committee (wwPDBAC), the members of the wwPDB have carried out the data uniformity project to overcome several historical problems, due to ambiguous definitions of terms and lack of mandatory information. In addition, PDBj has been engaged in improving the primary citation information. Finally, with standardized descriptions of atom names of macromolecules and ligands molecules, the wwPDB updated all the PDB data on August 1st, 2007, resulting in version 3[1)]. Version 3 is identified with "REMARK 4" in the PDB format, with the "_pdbx_version" category in the mmCIF format, and with the tag of "pdbx_versionCategory" in the PDBML format.

On September 7, 2007, the 7th wwPDBAC meeting was held at Princeton, USA, by the RCSB-PDB. The current situation and the future issues were presented and discussed by all the participants: The members of the wwPDB, Prof. Helen M. Berman (RCSB-PDB), Dr. Kim Henrick (MSD-EBI), Prof. Haruki Nakamura (PDBj), Prof. John L. Markley (BMRB), the AC members who are specialists in field 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, Prof. Angela M. Gronenborn, Dr. Gerard J. Kleywegt, Prof. Gaetano Montelione, Dr. Kei Yura, and Prof. Soichi Wakatsuki. In addition, as 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.

In this wwPDBAC meeting, it was intensively discussed how to increase the data quality. It was finally concluded that either the structure factors, in the case of X-ray crystallography, or the distance restraints, in the case of NMR experiments, should be simultaneously deposited with the atom coordinates as mandatory information. This conclusion was discussed in the international societies and approved, and was then announced to the Editors of major international journals. This new policy started on February 1st, 2008[2)].

The participants of the wwPDBAC meeting held on Sept. 7, 2008 at Princeton.

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

On September 9 and 10, 2008, the wwPDB Planning Retreat was also successively held. Dr. Takanori Matsuura (Associate Professor of Osaka Univ., PDBj), Ms. Reiko Igarashi (Primary annotator, PDBj), and Prof. Haruki Nakamura (PDBj) participated the Retreat, and had informal discussion with the other annotators and members of the wwPDB.

The next 5th wwPDBAC meeting will be held on September 29, 2008, at Hinxton, UK, by MSD-EBI.

References:

1) Kim Henrick, Zukang Feng, Wolfgang F. Bluhm, Dimitris Dimitropoulos, Jurgen F. Doreleijers, Shuchismita Dutta, Judith L. Flippen-Anderson, John Ionides, Chisa Kamada, Eugene Krissinel, Catherine L. Lawson, John L. Markley, Haruki Nakamura, Richard Newman, Yukiko Shimizu, Jawahar Swaminathan, Sameer Velankar, Jeramia Ory, Eldon L. Ulrich, Wim Vranken, John Westbrook, Reiko Yamashita, Huanwang Yang, Jasmine Young, Muhammed Yousufuddin and Helen M. Berman (2008) Remediation of the protein data bank archive. Nucl. Acids Res. 36, D426-D433.

2) John L. Markley, Eldon L. Urich, Helen M. Berman, Kim Henrick, Haruki Nakamura, Hideo Akutsu (2008) BioMagResBank (BMRB) as a partner in the Worldwide Protein Data Bank (wwPDB): new policies affecting biomolecular NMR deposition. J. Biomol. NMR, in press.

International Workshop: Computational and Experimental approaches to protein interactions and complexes

The International Workshop: Computational and experimental approaches to protein interactions and complexes, by JST (Japan Science and Technology Agency) and the Institute for Protein Research, Osaka University, was held on February 29th-March 1st. Approaches for computational structural bioinformatics, especially analysis of protein-protein interactions, were presented and discussed by invited experts in bioinformatics, computational biology and structural biology from home and abroad.

Snapshots of the Workshop.

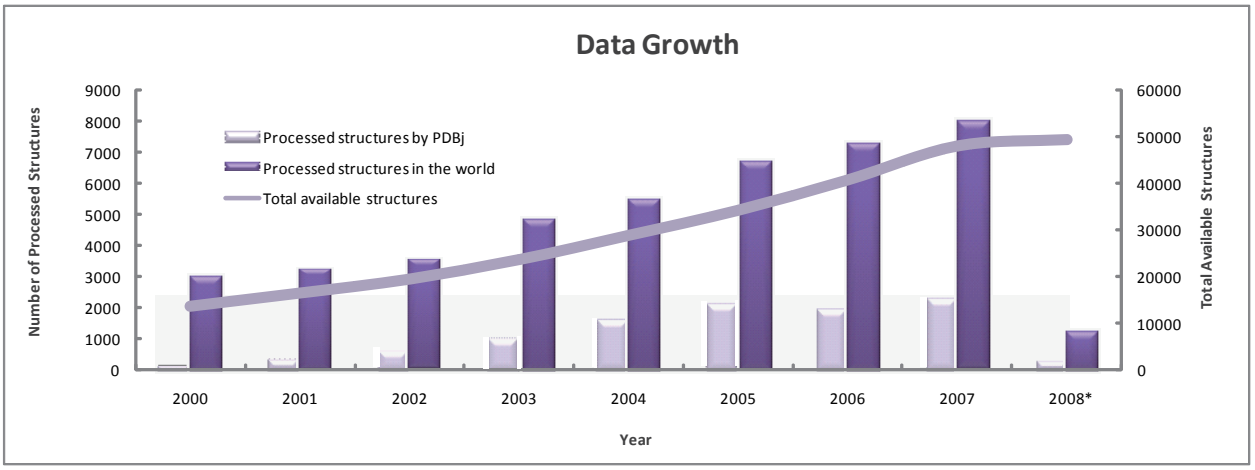
PDBj Workshop at Nakanoshima Center

The PDBj workshop was held at Osaka University, Nakanoshima Center on March 3rd, 2008. We introduced our services for participants. We got all sorts of comments from them about our services.

Snapshots of the Workshop.

Statistics

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



* Last updated : March 13, 2008

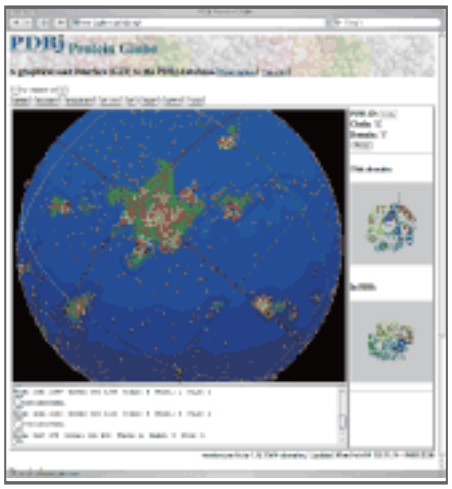
Services

XQuad: PDBML XQuery Advisor

An example of the XQuad page.

PDBj manages the data browsing system, xPSSS: xml-based Protein Structure Search Service, using the PDBML, which is a canonical XML description of the PDB data. As the advantage of the XML-Database, flexible and user-customized query services, XQuery and XPath, are available. However, without precise and correct understanding of the complicated schema of the PDBML, it is not easy to utilize those queries by XQuery or XPath. Therefore, we have recently developed a new service, XQuad (PDBML XQuery Advisor), to support to issue those queries for users who do not have much knowledge about the PDBML schema. PDBj plans to develop other web services, which are useful to users, with the advanced informatics technology.

Protein Globe



Protein Globe of example(1WXJ).

Protein Globe (the Globe) is an experimental graphical user interface to the PDBj services. The Globe visualizes the distribution of protein folds in the protein fold space: Each representative protein fold is represented as a point on a sphere and structurally similar folds are clustered together. Structural similarities were calculated by using the program ASH which is also provided by PDBj. Cartoon figures of some 50 most abundant folds are also mapped on the Globe so that a user can easily grasp the overall features the fold space. The user can select a fold by clicking the corresponding point on the Globe, and the information of the selected fold (PDB ID and cartoon figure) is displayed on the right column of the page for further visual inspection. Subsequently, the user can send the selected fold to other PDBj services such as xPSSS summary page to find more information of the entry, Sequence Navigator and Structure Navigator to find sequence and structural homologs, eF-site page to examine electrostatic and other surface properties of the entry. We are planning to elaborate the functionality of the Globe. Suggestions and comments are welcome.

Development of Sequence-Structure Integrated Multiple Alignment System

Our group is involved in a project entitled “Development of databases for folds, function, and evolution of proteins and their searching systems” in PDBj, which consists of three subprojects, (1) development of classification system of protein folds and the rapid searching with the classification, (2) development of sequence-structure integrated multiple alignment, and (3) construction of a database for evolutionary trace information. The persons in charge of the three subprojects are as follows; (1) Daron Standley (Osaka Univ.), (2) Kazutaka Katoh (Kyushu Univ.), (3) Hiroyuki Toh and Miki Ootsu (Kyushu Univ.). Here, I’ ll introduce the result of the second subproject, sequence-structure integrated multiple alignment.

Recent growth of protein structure database associated with the progress of structural genomics is quite rapid. Comparing to the number of available amino acid sequences, however, the number of proteins structures is still small. On the other hand, it is difficult to make an accurate alignment only from amino acid sequences, when the evolutionary distances are large among homologous proteins. Therefore, we have developed a system to construct an accurate and rapid multiple amino acid sequences alignment by integrating the information about amino acid sequences and tertiary structures. The “integration” here means that sequences are aligned under the constraint of structural alignment.

The output of a structural alignment program, GASH [1] (http://pdbjs3.protein.osaka-u.ac.jp/gash/run_gash.do), which has been developed by Dr. Standley, was used as an input of our system. By using the structural alignment as a constraint, a sequence-structur e multiple alignment was constructed with MAFFT [2, 3] (http://align.bmr.kyushu-u.ac.jp/mafft/software/). MAFFT was developed by Dr. Katoh when he belonged to the laboratory of Prof. Miyata of Kyoto University. MAFFT is now recognized as one of the most practical tool for multiple sequence alignment. The sequence-structure alignment system is available at the site, http://timpani.bmr.kyushu-u.ac.jp/~mash/.

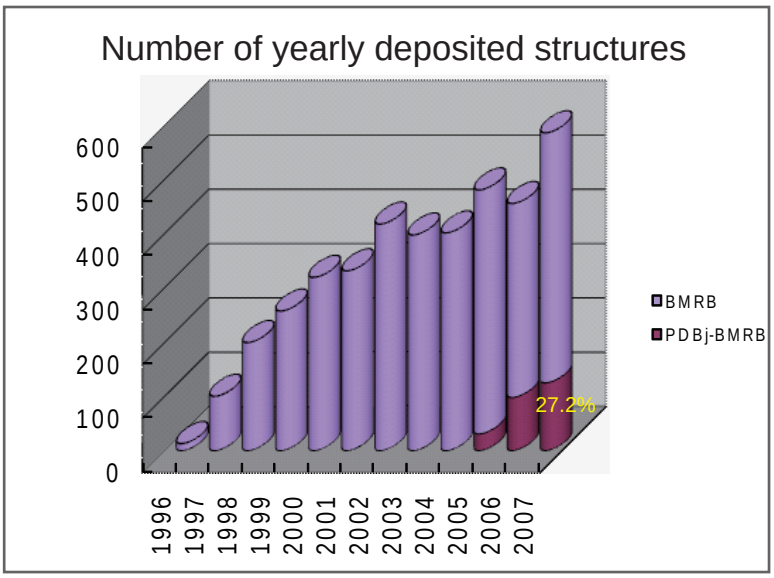
GASH is used in the current system as described above, since the format of the output suits MAFFT. However, RASH（http://pdbjs3.protein.osaka-u.ac.jp/rash/run_rash.do）, which has been also developed by Dr. Standley, is more accurate and rapid to construct a structural alignment than GASH. Substitution of GASH with RASH and introduction of other structural properties will be the next work to improve the performance of the sequence-structure integrated multiple alignment system.

[1] Stadley et al. (2005) BMC Bioinforatics 6, 211.
[2] Katoh et al. (2002) Nucleic Acids Res. 30, 3059.
[3] Katoh and Toh (2008) Briefings in Bioinformatics (in pess).

PDBj-BMRB Research and Development Report 2007

PDBj-BMRB collaborates with BioMagResBank (BMRB), at Wisconsin Univ. in Madison to develop an NMR database for proteins, peptides and nucleic acids. PDBj-BMRB assists in data deposition for NMR users, especially in Asian countries, and contributes to the broader scientific community as a valuable structural bioinformatics resource.

PDBj launched the mirror site for BMRB at the Institute for Protein Research, Osaka Univ., in March, 2002. Since then, the number of yearly deposits to the BMRB websites has steadily increased as shown in the following figure. Deposit to the Osaka site accounted for 27.2% of the total deposits to BMRB in 2007.



PDBj accepted 125 data depositions to the BMRB in 2007. This is twenty percent of the total number of BMRB depositions in 2007. This number is larger by about 10% than in 2006. About 70% of data entries came from RIKEN, Yokohama as part of the comprehensive NMR structural genomics National Project, Protein 3000. These data depositions are facilitated by data annotation through an intermediate data format designed especially for RIKEN. This procedure allows omitting ordinal manual data inputs through the ADIT-NMR interface.

In November, 2007, we released an enhanced Japanese website http://bmrbdep. protein.osaka-u.ac.jp. Here, a revised data deposition manual is available. As previously reported, this new site accepts the simultaneous depositions to PDB and BMRB through ADIT-NMR. This site provides a novel numerical program for chemical shift assignments and structural analysis based on spectral simulation developed by PDBj-BMRB (Y. Matsuki et al., J. Biomol. NMR 38, 325 (2007)). We also made a Korean and a Chinese BMRB websites in February, 2008.

In 2007 we presented BMRB activities through a number of conferences, such as the annual meetings of the protein science society, the biophysical society, the NMR society of Japan, and the Asia-Pacific NMR symposium, which has helped to promote the presence of PDBj-BMRB in the biological NMR community.

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
FAX: +81-(0)6-6879-8636
URL: http://www. pdbj.org/

Director
Prof. Haruki Nakamura (IPR, Osaka University)