PDBj
Protein Data Bank Japan
http://pdbj.org/

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PDBj, wwPDB, and their activities

In July 2000, the Protein Data Bank Japan (PDBj, http://pdbj.org/) at the Institute for Protein Research (IPR), Osaka University, started accepting new structures of biological macromolecules from researchers mainly in Asia and Oceania regions, and processed them for the common PDB data having high qualities. Since then, the PDBj has become the representative archive of this region, as one of the four members of the wwPDB (worldwide PDB, http://wwpdb.org/) (Fig.1). The PDBj has also developed several characteristic web services and provided them freely to the structural biologists and bioinformatics in the world. In addition, PDBj-BMRB (BioMagResBank) group was founded in PDBj at the early days so as to process and edit the chemical shifts information collaborating with BMRB in USA. These activities of the PDBj are now supported by JST-NBDC (Japan Science and Technology Agency - National Bioscience Database Center, http://biosciencedbc.jp/), and Osaka University.

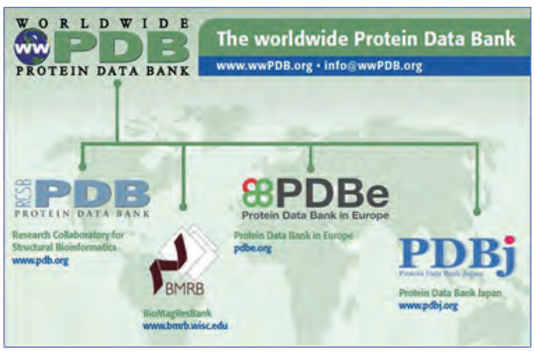


Fig.1: The worldwide PDB

Every year, the wwPDB registers more than 10,000 structures of biological macromolecules such as proteins and nucleic acids, determined all over the world for a total of over 114,000 structures as of December 2015. So far, PDBj has processed about 22 % of the entries, collaborating with the other wwPDB members: the RCSB-PDB in USA, the PDBe-EBI in the EU, and the BMRB (BioMagResBank). The members gather frequently to discuss current issues and the future progress of the wwPDB.

The First wwPDB/CCDC/D3R Ligand Validation Workshop

The First wwPDB/CCDC/D3R Ligand Validation Workshop was held on July 30-31st, 2015 at Rutgers University, NJ, USA where co-crystal structure determination experts from academe and industry with X-ray crystallography and computational chemistry software developers were invited (Fig.2).

In this workshop, after a Keynote presentation was made by Dr. Cathy Peishoff from GSK, four small groups discussed the following issues: What data concerning ligands should be archived? How should the ligands be best represented? How should the structures of protein-ligand complexes be validated? What information should accompany the publication of protein-ligand complex structure?

Finally, all the participants discussed together and developed consensus recommendations. A white paper has been written, and it will soon be published.

Fig.2: Participants of the first wwPDB/CCDC/D3R Ligand Validation Workshop at Rutgers University, NJ, USA

The 12th wwPDB Advisory Committee meeting

The wwPDB (worldwide Protein Data Bank), of which the PDBj is one of the members, organizes the annual advisory Committee (wwPDBAC) meeting every year. In 2015, we, PDBj, hosted the 12th meeting on October 2, 2015, at Institute for Protein Research (IPR), Osaka University. The participants were Prof. R. Andrew Byrd as a chair (National Cancer Institute at Frederick), Prof. Stephen K. Burley, Dr. John Westbrook and Dr. Jasmine Young (RCSB-PDB, Rutgers Univ.), Dr. Sameer Velankar (PDBe, EBI), Dr. Rolf Apweiler (EBI), Prof. John L. Markley (BMRB, Univ. Wisconsin-Madison), Prof. Haruki Nakamura (PDBj, Osaka Univ.), Prof. Paul Adams (Lawrence Berkeley National Laboratory), Prof. Cynthia Wolberger (Johns Hopkins Univ.), Prof. Helen Saibil (Birkbeck College London), Prof. David Brown (Univ. of Kent), Prof. Genji Kurisu (IPR, Osaka Univ.), Prof. Daisuke Kohda (Kyushu Univ.), Prof. Wah Chiu (Baylor College of Medicine) as an EM Representative, Prof. Edward Baker (Auckland Univ.) as a representative of IUCr, and Prof. Angela M. Gronenborn (Univ. of Pittsburgh) and Prof. Masatsune Kainosho (Tokyo Metropolitan University) as representatives of BMRB. In addition, Prof. Jianping Ding (Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, China) and Prof. Manju Bansal (Indian Institute of Science) attended the meeting as the associated member (Fig. 3).

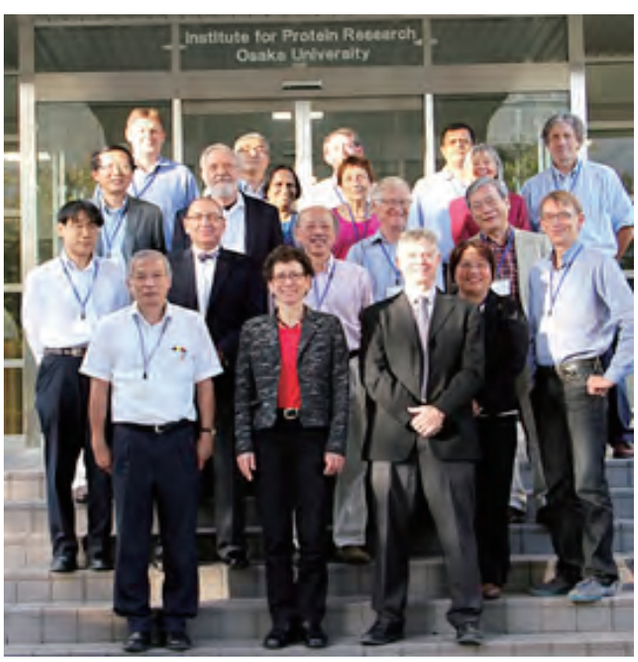


Fig.3: Participants of the 12th wwPDBAC meeting at IPR, Osaka Univ.

After an overview and an introduction of the out-reach activities were made by Prof. Haruki Nakamura in PDBj, the progress of Common Deposition and Annotation (D & A) program was introduced and its current software system was shown by Prof. Stephen K. Burley, representing the team developing the Common D & A program.

Next, the updates of the BMRB funding, staffing, and depositions statistics were introduced by Prof. John L. Markley. The report for the wwPDB NMR Validation Task Force held in January 2015 was introduced, in particular, with the information and current details of NMR Exchange Format (NEF).

Because the head of PDBe, Dr. Gerard Kleywegt, was absent, Dr. Sameer Velankar introduced the current situation of the EMDB (Electron Microscopy Data bank) and EMPIAR (Electron Microscopy Pilot Image Archive), with the validation issues for EM data.

In this wwPDBAC meeting, some delay was pointed out for the development of D&A (Deposition and Annotation system) version 2.0, in which all the NMR and EM data in addition to X-ray crystallographic data can be deposited by the researchers, and annotated by the wwPDB annotators with the data validations. The progress and updated roadmap were critically discussed, and the public release was re-scheduled in January 2016. For that time line, strong collaboration among all the four wwPDB members is highly appreciated.

In addition, several new issues were discussed: 1) the wwPDB is going to capture an ORCID (Open Researcher and Contributor ID) for each contact author at the time of deposition, 2) the wwPDB is going to adopt the principles guiding Federation of data resources with the PDB archive for the purpose of supporting PDB archive deposition, annotation, validation, and distribution of Integrative/Hybrid 3D structural models, and 3) the wwPDB is going to introduce a new versioning system.

Finally, it is announced that the next wwPDBAC meeting will be held at the beginning of October 2016 at University of Wisconsin-Madison, USA.

The wwPDB Symposium

The wwPDB Symposium on Integrative Structural Biology with Hybrid Methods was held on 3 October 2015 at Osaka University Hall, Auditorium (Fig. 4). It focuses on the multi-scale structural biology, which aims to analyze structures of protein molecules and their assemblies, cellular machines, organelle, and even living cells and organisms by the hybrid methods, integrating many different technologies, such as chemical cross-links, MS spectrometry, FRET, Super-resolution microscopy, X-ray diffraction, NMR, and Computer modeling, in addition to Cryo-EM that has been attracting much attention these days.

Fig.4: The poster of the wwPDB Symposium on Integrative Structural Biology with Hybrid Methods, held on 3 October 2015.

After an opening remark made by Prof. Haruki Nakamura in IPR, Osaka University, by 12 invited speakers to the symposium, their researches with the hybrid methods were introduced, and construction of a new database with data validation and putative applications to drug discovery were discussed (Figs. 5 and 6). Finally, Prof. Stephen K. Burley addressed a closing remark, emphasizing the important roles of the wwPDB. There were totally 93 attendees, including the speakers and audience, and many exciting latest topics were introduced.

This Symposium was held as an outreach of the wwPDB Foundation (The worldwide Protein Data Bank Foundation) for its educational and social contributions.

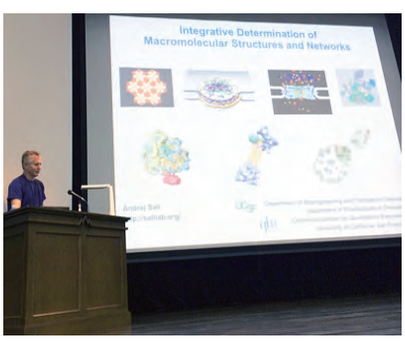


Fig.5: The invited talk by Prof. Andrej Sali from UCSF.

Fig.6: The invited talk by Prof. Helen M. Berman from Rutgers Univ. (Left), chaired by Prof. John L. Markley from Univ. Wisconsin-Madison (Right).

Topics

wwPDB Deposition and Annotation System version 2.0

At the beginning of January 2016, a new deposition and annotation system (D&A) version 2.0 will start for structures determined using 3DEM (3-Dimensional Electron Microscopy) or NMR (Nuclear Magnetic Resonance). The new system interoperates with EMDB and BMRB to enable joint depositions of both atomic coordinates (PDB) and electron density maps (EMDB) or NMR experimental data (BMRB). Both PDB and EMDB/BMRB accession codes are issued simultaneously. In addition, D&A version 2.0 will include generation of validation reports for the structures determined not only by X-ray crystallography but also NMR and EM.

For at least the first half of the year 2016, depositors will have the option of using the new system or one of the legacy deposition tools (EM-Dep, ADIT-NMR, AutoDep) to start a new deposition. Once the new system is deemed stable, the legacy deposition tools will be phased out with sufficient time allowed for completion of unfinished sessions.

Seeking 3DEM and SAS structures by Omokage search

http://pdbj.org/emnavi/omo-search.php

We added data in another type to Omokage search *1, which is the similarity search tool based on shapes of biological molecules. In order to cross-search of structural data, atomic models and 3D density maps, the search system considers only similarities of global shapes of the structures, and ignores whether they are proteins, RNAs, or unknown masses of coulomb potential. In addition to the PDB atomic models and EMDB density maps, structure models deposited in Small Angle Scattering Biological Data Bank (SASBDB)*2 are included to the search database. Now, Omokage search can cross-search the three databanks. While SASBDB is a databank for SAS profile data, three types of structure data, dummy atom models, atomic models, and mixtures of both, are stored additionally. Just by inputting ID of the model in the Omokage search page, the user can start the search. Similar shaped structural data from the three databanks will appear as the search result (Fig.7).

By recent innovation called "resolution revolution" , 3D electron microscopy (3DEM) is growing to be an atomic-model determination method comparable to X-ray crystallography and NMR, and the number of EMDB entries is rapidly increasing. On the other hand, according to growth in demand of structural information of flexible biomolecules in solution, BIOISIS and SASBDB were established to share SAS data. Number and variety of biomolecule' s structure data out of the range of PDB will continue to increase. We, PDBj, will also concern to deal such the complication of structural data by providing services such as Omokage search.

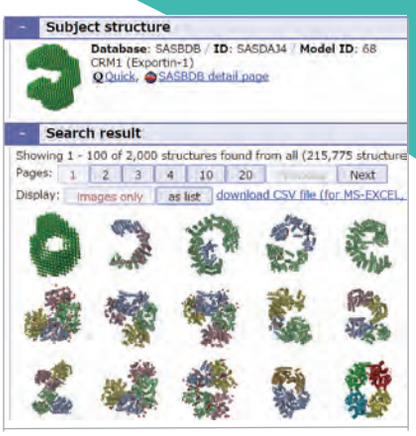


Fig.7: Example of search using SASBDB data

*1: Suzuki H, Kawabata T, Nakamura H. Omokage search: shape similarity search service for biomolecular structures in both the PDB and EMDB. Bioinformatics. 2015 btv614.

*2: SABDB: http://www.sasbdb.org/

PDBj-BMRB

PDBj-BMRB group has published XML and RDF documents of biomolecular NMR data archived at BioMagResBank (BMRB), which allows users to gain the information related to the entry such as chemical shifts, structure coordinates, function and interaction of proteins, and single nucleotide polymorphism (SNP). Using the BMRB/RDF via SPARQL endopoint, PDBj-BMRB group has established secondary database of modeled structures for the human genome (SAHG) linked with the other life science databases.

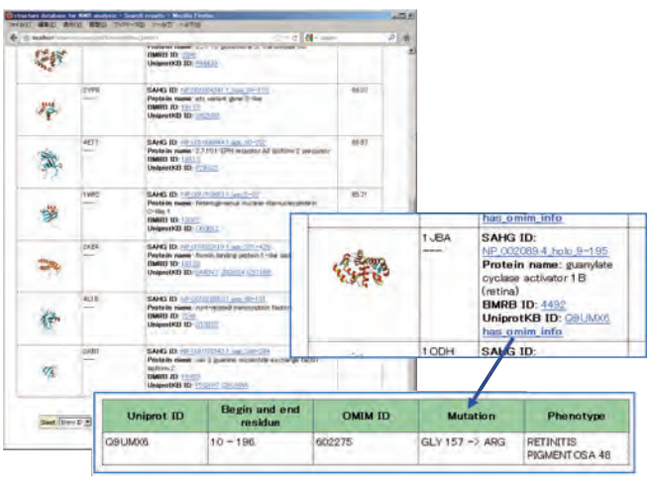


Fig.8: Secondary database of modeled structures using XML and RDF

NMR Validation Task Force metting in Rutgers University

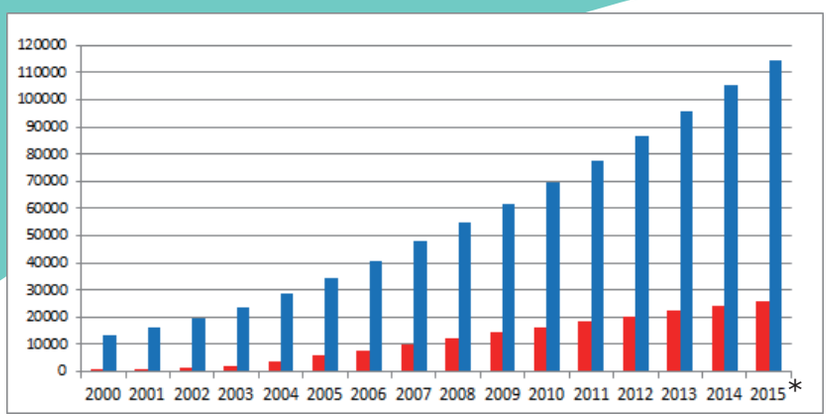
Fig.9: NMR VTF meeting in Rutgers University

One of the members of PDBj-BMRB group has attended NMR Validation Task Force (NMR-VTF) meeting which was held in Rutgers University at Jan. 2015 (Fig.9). In the meeting, new exchange format for NMR restraint has been established as NEF format and published to Nat. Struct. Mol. Biol. at June 2015 *3.

*3: NMR Exchange Format: a unified and open standard for representation of NMR restraint data. Gutmanas A., Adams P. D., Bardiaux B., Berman H. M., Case D. A., Fogh R. H., Güntert P., Hendrickx P. M., Herrmann T., Kleywegt G. J., Kobayashi N., Lange O. F., Markley J. L., Montelione G. T., Nilges M., Ragan T. J., Schwieters C. D., Tejero R., Ulrich E. L., Velankar S., Vranken W. F., Wedell .

Data Growth

The statistics data are also available at the wwPDB web page;
http://wwpdb.org/stats.html



*As of December 30, 2015

Event Report

The Activities done for introducing PDBj and our web services.

- Osaka University ICHO festival -Exbition for Protein Structure by 3D viewer
  (May 2, 2015, Institute for Protein Reseach)
- PDBj & Plattform for Drug Dicovery, Informatics and Structural Life Science Joint Wokshop for the Databases (*June 13, 2015, JST, Tokyo, Japan)*
- Luncheon Seminar at the 15th Annual Meeting of the Protein Science Society of Japan (*June 24, 2015, Tokushima, Japan)*
- The First "All-in-One" joint workshop for the life science data bases
  (July 18, 2015, Osaka, Japan)
  by NBDC (National Bioscience Database Senter, DDBJ (DNA DataBank of Japan), DBCLS (Database Center for Life Science), and PDBj
- Luncheon Seminar at the 53th Annual Meeting of the Biophysical Society of Japan *(September 13, 2015, Kanazawa, Japan)*
- Luncheon Seminar at the Annual Meeting 2015 of Crystallographic Society of Japan *(October 18, 2015, Osaka, Japan)*
- Luncheon Seminar at the 4th Joint Conference on Informatics in Biology, Medicine and Pharmacology
  (October 29, 2015, Kyoto, Japan)
- Science Agora 2015 - The Scientific Events Supported by JST.
  (November 13-15, 2015, Tokyo)

At the Icho festival on May 2, 2015

The Luncheon Seminar on Oct 18, 2015

The workshop on June 13,2015

The Science Agora, Nov 13-15, 2015

- Exbition Booth and Presentation for the Databases at the 38th Annual Meeting of the Molecular Biology Society of Japan
  (December 1-3, 2015, Kobe, Japan)

Seminar and Workshop Materials are Available for Download;
http://pdbj.org/info/previous-workshop

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