

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/>). 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.

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 125,000 structures as of December 2016. 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. The members gather frequently to discuss current issues and the future progress of the wwPDB.

Joint NMR VTF and NEF Workshop

Joint NMR VTF (Validation Task Force) and NEF (NMR Exchange Format) Workshop was held on August 26-27th at Institute for Protein Research (IPR), Osaka University, to establish the description method of NMR experimental data.

The atomic structure determination by NMR experiments requires the distance restraints between the spin pairs of atomic nuclei and the dihedral angles in a molecule, which are also essential to validate the consistency between the atomic structural model and the NMR experiments. In order to establish the description format for the above experimental information, BMRB with the NMR-VTF members, who have developed the NMR-STAR format, and the NEF group members gathered together at IPR, Osaka University just after ICMRBS-2016 international congress held in Kyoto, and they had a joint workshop. The hosts of this workshop were Prof. J. L. Markley (Univ. of Wisconsin-Madison), Prof. H. Nakamura (IPR, Osaka Univ.), and Prof. T. Fujiwara (PDBj-BMRB, Osaka Univ.). The other attendees were A. Bax (NMR-VTF), R. A. Byrd (NMR-VTF), P. Güntert (NMR-VTF, NEF), T. Herrmann (NMR-VTF, NEF), G. T. Montelione (NMR-VTF, NEF), M. Nilges (NMR-VTF, NEF), T. Polenova (NMR-VTF), C. Schwieters (NMR-VTF, NEF), N. Sgourakis (NEF), G. W. Vuister (NMR-VTF, NEF), S. Velankar, A. Gutmanas (PDBe), S. K. Burley, J. Westbrook (RCSB-PDB), K. Baskaran, P. Romero (BMRB), and N. Kobayashi (PDBj-BMRB). There were total 20 attendees including the hosts (Fig. 1).

In this workshop, there were five sessions. After introduction of the current situations of both the NEF and NMR-STAR, all the participants discussed the following issues: How to interconvert

the data between NEF and NMR-STAR? How should the structures be validated and the validations be reflected on the Validation reports? How should the experimental information be implemented as the input data in the OneDep program?

Finally, the role of each developer for the new common standard was proposed with priority. The timelines were also shown for developments of dictionaries and tools for interconversion of the data in NEF and NMR-STAR formats so that the developers will be able to follow.



Fig. 1: Participants of the Joint NMR VTF and NEF Workshop at IPR, Osaka University on August 26-27th 2016.

NII Shonan meeting on Web-based Molecular Graphics

The NII Shonan meeting on Web-based Molecular Graphics was held on September 5-8th 2016 at Shonan village, Kanagawa prefecture by the three organizers: Prof. Haruki Nakamura (PDBj, Osaka Univ.), Prof. Seán I. O' Donoghue (CSIRO & Garvan Institute, Australia), Dr. Andrea Schafferhans (TUM & HSWT, Germany) (Fig. 2). Total 28 attendees including the organizers made their own presentations and the group discussions for the following issues about the future technology of the web-based molecular graphics (Fig. 3): Augmented Reality and Virtual Reality/Building Mash-Ups – Interoperability Requirements/Mesoscale and Intermediate Representations/3D Rendering and Representation of Molecular Structures/ User Experience Best Practice/Chemoinformatics/Review of the State of the Art.

Researchers from the all wwPDB members attended this meeting, and they introduced the methods to rapidly access the information of large structures and the core technologies for their visualization. Thus, it was impressed that the wwPDB members' technologies lead the world in this field.



Fig.2: Organizers of the NII Shonan meeting (From left to right, Prof. Haruki Nakamura, Dr. Andrea Schafferhans, and Prof. Seán I. O' Donoghue)



Fig.3: The attendees of the NII Shonan meeting on Web-based Molecular Graphics held on September 5-8th 2016.

The 13th wwPDB Advisory Committee meeting

The wwPDB (worldwide Protein Data Bank), of which the PDBj is one of the members, organizes the annual advisory Committee (wwPDB AC) meeting every year. This year, BMRB hosted the 13th meeting on October 7, 2016, at University of Wisconsin-Madison. 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), 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. Sarah Butcher (Helsinki Univ.), Prof. David Brown (Univ. of Kent), Prof. Genji Kurisu (IPR, Osaka Univ.), Prof. Tsuyoshi Inoue (Osaka Univ.), Prof. Wah Chiu (Baylor College of Medicine) as an EM representative, Prof. Edward Baker (Auckland Univ.) as a representative of IUCr, and Prof. Arthur Edison (Univ. of Georgia) and Prof. Valérie Copié (Montana State Univ.) as a representatives of BMRB. In addition, Prof. Manju Bansal (Indian Institute of Science) attended the meeting as the associated member. Dr. John Westbrook (RCSB-PDB), Dr. Rolf Apweiler (EBI) and Dr. Gerard Kleywegt (EBI) also participated in the meeting as an Observer (Fig. 4).

In the wwPDB AC meeting, the wwPDB PIs (Prof. John L. Markley (BMRB), Prof. Stephen K. Burley (RCSB-PDB), Dr. Sameer Velankar (PDBe), and Prof. Haruki Nakamura (PDBj)) and Dr. Jasmine Young as the project leader of OneDep introduced the activities of the wwPDB, and its future was discussed.

After an overview made by Prof. John L. Markley, the progress of the OneDep as the new pipeline of Common Deposition, Annotation, and Validation program was introduced by Dr. Jasmine Young (RCSB-PDB). In particular, she finally introduced an announcement from Editorial of "Nature Structural & Molecular Biology" in October issue 2016 that they are requesting official wwPDB validation reports for peer review and that other Nature journals will soon follow suit. This policy change in Nature journals is expected to be extended in

many other journals in the near future. Usage of ORCID ID for identifying the authors and of versioning system with the change of the current four characters of PDBIDs were also introduced and discussed.

Next, Prof. Haruki Nakamura introduced the wwPDB outreaches: Symposia, International meetings such as the NII Shonan meeting mentioned above, and Promotion of the PDB and structural biology. Prof. Stephen K. Burley showed the progress of the deposition, annotation and validation of the X-ray crystal structures. He also announced starting a new trial of the group deposition, where 364 structures were processed with the group ID "G_1002001". Dr. Sameer Velankar (PDBe) introduced the current rapid increase of atomic structures derived from the cryo-EM and their validations. Prof. John L. Markley (BMRB) introduced the current activities of BMRB, and, in particular, about the Joint NMR VTF (Validation Task Force) and NEF (NMR Exchange Format) Workshop, which was held on August 26-27th 2016.

Finally, it has been announced that the next wwPDB AC meeting will be held on October 6th 2016 at Center for Integrative Proteomics Research, Rutgers University, USA.



Fig. 4: Participants of the 13th wwPDB AC meeting at BMRB in University of Wisconsin-Madison on October 7th 2016.

Publication and application of NMR database in XML and RDF

PDBj-BMRB group has developed tools for conversion of NMR data in BioMagResBank (BMRB) and released SPARQL endpoint (Yokochi et al., J. Biomed. Sem. 2016, 7(16)). We have also opened a new portal web-page implemented with highly sophisticated search function to obtain a wide variety of data including sequence, structure, NMR data, protein-protein interaction by database search of PDB, BMRB, UniProt and IntAct.

Release of new version of integrated NMR analysis tool, MagRO

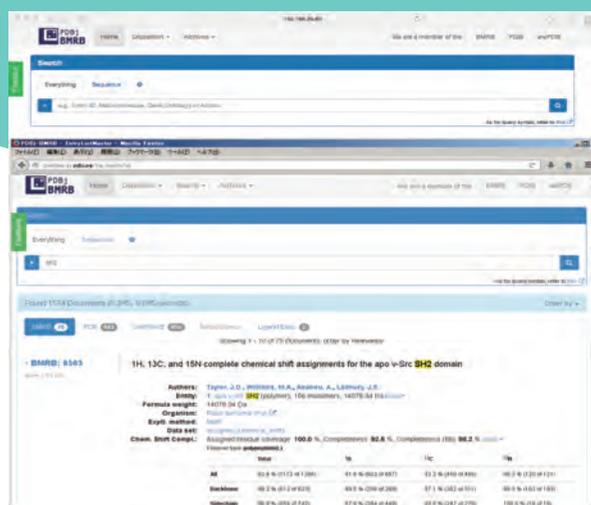


Fig.7: New portal web-page with new database search function

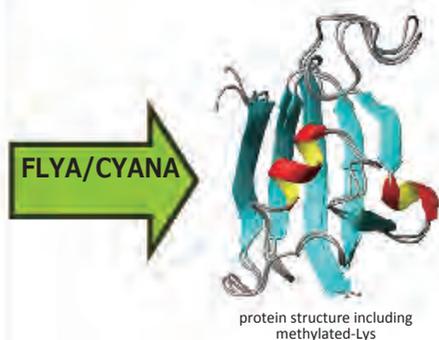
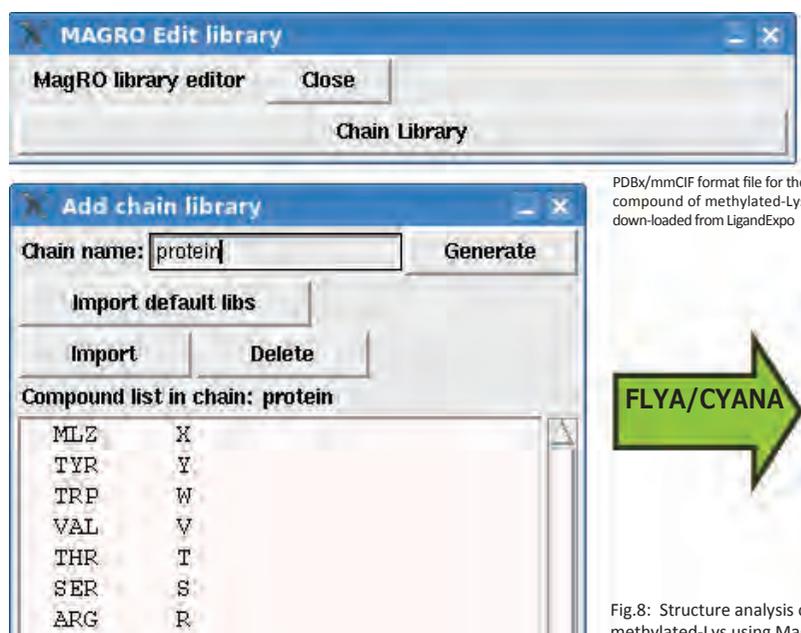


Fig.8: Structure analysis of protein including methylated-Lys using MagRO, FLYA/CYANA

PDBj-BMRB has developed and released new version of integrated NMR analysis tool, MagRO (ver. 1.37.0x) for a highly-automated NMR data analysis (Kobayashi et al., ICMRBS2016, Kyoto).

The new version has a function to import chemical compound data in PDBx/mmCIF format from the database such as LigandExpo and to assist the NMR signal assignments and structure calculation with FLYA/CYANA.

The 14th International Conference of Asian Crystallographic Association (AsCA 2016)

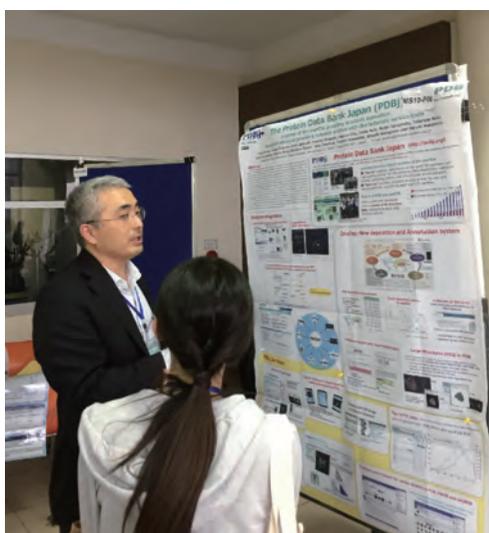


Fig.9: Poster presentation at AsCA 2016

The Asian Crystallographic Association Meeting (AsCA) was held in Hanoi, Vietnam, from December 4th to 7th, 2016. Prof. Wah Chiu, who is an advisory board member to the world-wide PDB, gave us an impressive talk on the recent results of cryo-TEM analysis. Throughout the whole meeting, I realized that Hybrid method including Cryo-TEM start emerging also in the Asia and Oceania. PDBj had a poster presentation entitled "The Protein Data Bank Japan (PDBj): A partner of the wwPDB accepting structure deposition through OneDep and providing common archive with characteristic service tools". We introduced our new deposition tools named "OneDep", new Validation reports and future plan of PDB-ID versioning to the biological crystallographers from Asia and Oceania. The international program committee of AsCA' 16 assigned our poster presentation in the micro-symposium of "Hybrid Method". During our presentation, some comments and questions were came up from the attendees, mainly concerning about the batch-deposition and specific web searching. It must be important for PDBj to keep in touch with AsCA, as one of the scientific societies closely related to PDB activities. (Genji Kurisu, Osaka University)



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

■ Total available structures ■ Processed structures by PDBj

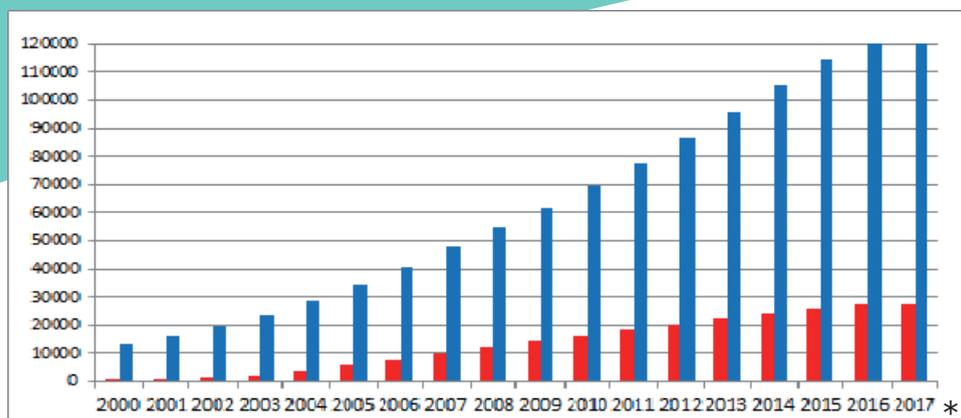


Fig.10

*As of January 25, 2017

Event Report

-The Activities done for introducing PDBj and our web services in 2016.

Osaka University ICHO festival -Exhibition for Protein Structure by 3D viewer
(May 1, 2016, Osaka, Japan)

PDBj & JAICI Joint Luncheon Seminar
at the 16th Annual Meeting of the Protein Science Society of Japan
(June 7, 2016, Fukuoka, Japan)

The "All-in-One" Joint Workshop
-How to Use Bio Data in Life Science Databases
(Jul 23, 2016, Osaka, Japan)

by NBDC (National Bioscience Database Center, DDBJ (DNA DataBank of Japan),
DBCLS (Database Center for Life Science), and PDBj

Joint NMR VTF and NEF Workshop
(August 26-27, 2016, Osaka, Japan)

PDBj Luncheon Seminar at the 5th Joint Conference on Informatics
in Biology, Medicine and Pharmacology (October 1, 2016, Tokyo, Japan)

Science Agora 2016 - The Scientific Events
Supported by Japan Science and Technology Agency
(November 3-6, 2016, Tokyo, Japan)

PDBj Luncheon Seminar at the Annual Meeting 2016 of
Crystallographic Society of Japan
(November 18, 2016, Ibaragi, Japan)

PDBj Luncheon Seminar
at the 54th Annual Meeting of the Biophysical Society of Japan
(November 25, 2016, Ibaragi, Japan)

Exhibition Booth for the Life Science Databases
at the 39th Annual Meeting of the Molecular Biology Society of Japan
(November 30 -December 2, 2016, Yokohama, Japan)



at ICHO festival



The "All-in-One" Joint Workshop



Luncheon Seminar at CrSJ 2016



Science Agora 2016



Luncheon Seminar at BSJ 2016

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

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