Protein Data Bank Japan

http://pdbj.org/

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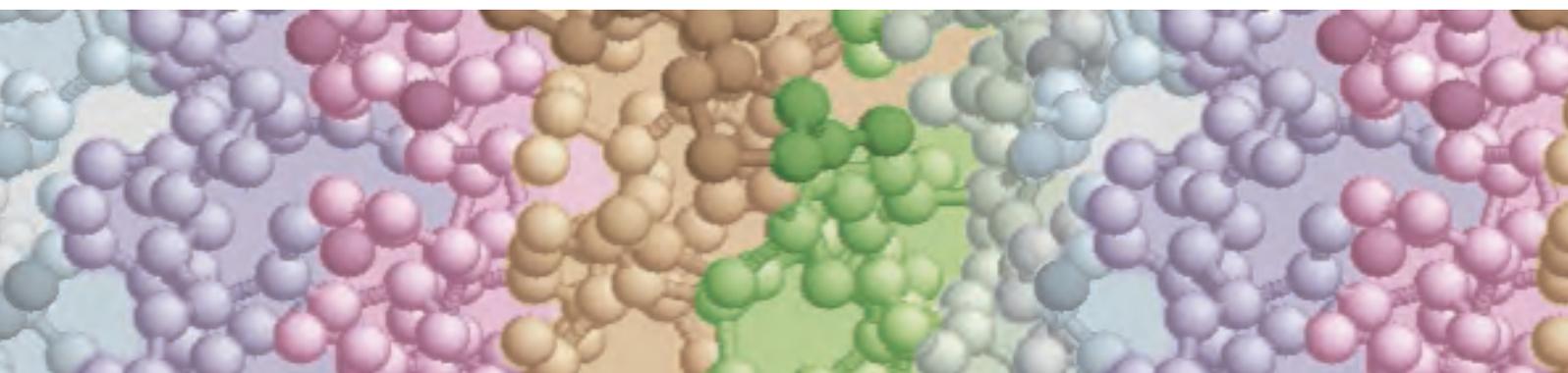
NEWS

The 9th 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. This year, we, PDBj, were a host, and the 9th meeting was held on October 12, 2012. The participants were Prof. Soichi Wakatsuki as a chair (KEK, Photon Factory), Prof. Haruki Nakamura (PDBj, Osaka Univ.), Prof. Helen M. Berman, Dr. Martha Quesada (RCSB-PDB, Rutgers Univ.), Dr. Gerard Kleywegt (PDBe, EBI), Prof. John L. Markley (BMRB, Univ. Wisconsin-Madison), Prof. Stephen Burley (UCSF), Prof. Michael Rossmann (Purdue Univ.), Prof. Guy Montelione (Rutgers Univ.), Prof. Wayne Hendrickson (Columbia Univ.), Prof. Cynthia Wolberger (Johns Hopkins Univ.), Prof. Helen Saibil (Birkbeck College London), Prof. Titia Sixma (Netherlands Cancer Inst.), Prof. Genji Kurisu (IPR, Osaka Univ.), Prof. Keiichi Namba (Osaka Univ.), Prof. Masatsune Kainosho (Nagoya Univ.), Prof. Edward Baker (Auckland Univ.) as a representative of IUCr, and Dr. R. Andrew Byrd (Center for Cancer Research, NCI) as a representative of ICMRBS. In addition, Prof. Jianping Ding (Shanghai Institutes for Biological Sciences, Chinese Academy of Sciences, China) attended the meeting as the associated member. Prof. Atsushi Nakagawa (IPR, Osaka Univ.) also participated the meeting as an observer from the PDBj (Fig. 1).

At the beginning of the meeting, the all wwPDB members gave a plaque to Prof. Stephen Burley, appreciating for his long and great efforts as a chair of the wwPDBAC. Then, the progress of Common Deposition and Annotation (D & A) program was introduced by Dr. Martha Quesda, and the beta-version was shown by a movie, how to deposit the data and to process it by the annotators in the web-based D & A system. Next, as previously agreed by the wwPDBAC members, the conventional PDB format will be updated based on the PDBx format. An actual format will be fixed at the beginning of the next year. PDBj has developed a new tool to validate the data description for the new format, and the PDB/RDF format, which is now distributed as a standard one from the wwPDB. In the last year, the report made by Validation Task Forces (VTFs) for X-ray crystallography in order to keep the data qualities was introduced. This year, the report for EM was published in Structure, and those for NMR and small-angle X-ray and Neutron scattering observations (SAXS/SANS) are now in progress.

The wwPDB Charter was agreed ten years ago, in 2003, and so a new Charter should be prepared and agreed in 2013. In addition, the wwPDB organization will also be reformed following an updated Terms of Reference for the wwPDB Advisory Committee, where the memberships and chairman ships should be clearly described.

The current funding for the RCSB-PDB will be ended at the end of 2013, and that for the PDBj will be ended at the end of March, 2014. It is also noticed that the BMRB funding situation is not very established. More fund raising efforts were discussed.

In summary, continuous efforts of the wwPDB members for the Common D & A program and establishment of the new PDBx format were appreciated.
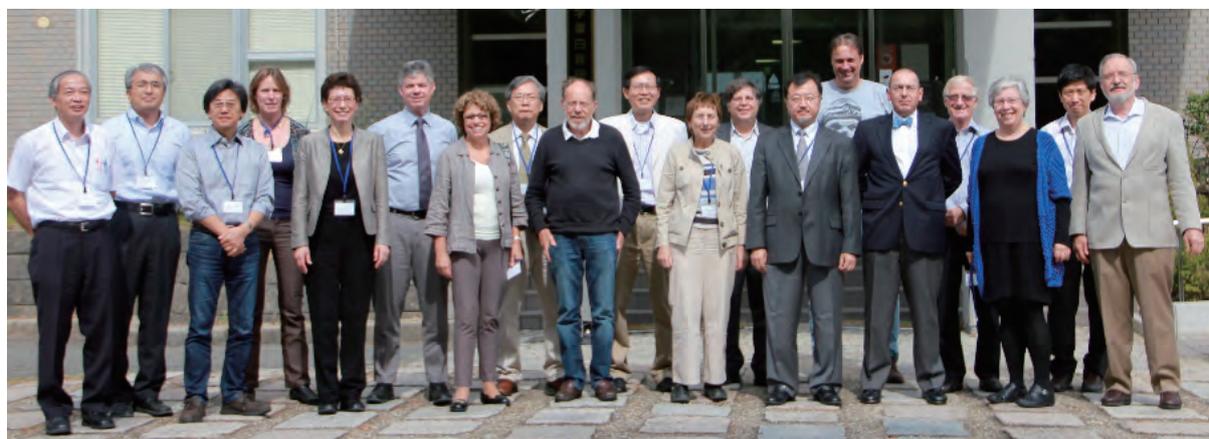
Fig. 1: Participants of the 9th wwPDBAC meeting at the Institute for Protein Research, Osaka University, on October 12, 2012.

wwPDB Foundation Outreach Seminar.
Protein Data Bank: Basis for Life Science and Drug Development

The wwPDB Foundation was founded in February 2010 by the wwPDB members. Last year, on October 28-30, 2011, PDB40 symposium was held at Cold Spring Harbor Laboratory, commemorating the 40th anniversary of the PDB by the wwPDB foundation. The purpose of this foundation is to promote the public interest in PDB and structural biology. This year, just after the 9th wwPDBAC meeting in Osaka University, an Outreach Seminar "Protein Data Bank: Basis for Life Science and Drug Development" was held at Hearton Hall, Umeda (Osaka city center), on October 13 (Saturday) 2012.

  At the seminar, three lectures were made: "wwPDB and its Impacts to Science and Society" by Prof. Haruki Nakamura (Institute for Protein Research, Osaka University), "Impact of the Protein Data Bank on Drug Discovery" by Prof. Stephen K. Burley (University of California at San Diego), and "Molecular Nanomachines in Living Organisms - Exquisite Structural Design far beyond State-of-the-Art Nanotechnology" by Prof. Keiichi Namba (Graduate School of Frontier Biosciences, Osaka University). Total 52 audiences including two high-school students listened the lectures enthusiastically and asked many questions to the lecturers (Fig.2). The slides used in the lectures are available from the web site (http://pdbj.org/pdbj_prev_workshop.html), and the part of the lectures can be seen on the YouTube.


Fig.2: wwPDB Foundation Outreach Seminar

Data Growth

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

■ Processed structures by PDBj
■ Total available structures
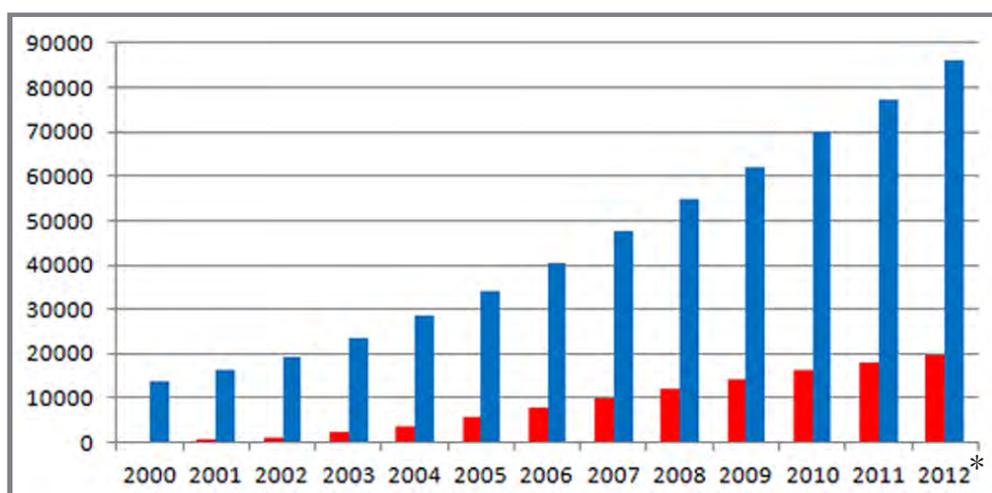
Fig.3   *As of November 14, 2012

EVENT ─Luncheon Seminar

PDBj introduced our recent activities and newly developed web services at luncheon seminars below;

◆**The 12th Annual Meeting of the Protein Science Society of Japan** (Jun 20 -22, Nagoya Congress Center)
・Development and Database Integration in PDBj（Protein Data Bank Japan）: Haruki Nakamura
・Web services at PDBj : Akira R. Kinjo
・Introduction of virtual computing for studies on biopolymers: techniques using virtual machines and support tools for data analysis and deposition. : Naohiro Kobayashi

◆**The 50th Annual Meeting of the Biophysical Society of Japan**（BSJ50）(Sep 22-24, Nagoya University)
・Roles of wwPDB and PDBj towards Big Data Era: Haruki Nakamura
・The integrated analysis platform for NMR data using virtualization technology: Naohiro Kobayashi

◆**The Annual Meeting of the Crystallographic Society of Japan** (Oct 25-26, Tohoku University)
・Activities of PDBj and wwPDB: Haruki Nakamura
・Data deposition to Protein Data Bank (PDB): Atsushi Nakagawa

─PDBj Workshop in Fukuoka

PDBj holds workshops in different areas of Japan periodically, for the purpose of education and training of database users, and took place at Maidashi Campus, Kyushu University in Fukuoka this year.


Fig.4:PDBj Workshop in Fukuoka

Service

Sequence to Function Annotation Service (SFAS)

SFAS is a web server that automates many of the common tasks in structure-based function prediction. Moreover, SFAS makes use of composition-based function prediction methods for regions of intrinsic disorder [1, 2]. This article will describe the steps involved in running SFAS for a typical query.

By default, the first step is to carry out "2D prediction". This will predict regions of intrinsic disorder and secondary structure. This helps us to select regions of interest for threading: that is, putative structural domains. Results are displayed as a graph (Fig.5) on which sub-sequences can be selected by dragging the mouse over the region of interest. The selected sub-sequence can then be submitted to our internal "meta threading server". The results of the threading calculations can be viewed or rendered as 3D models using Spanner [3]. The Spanner models can then be submitted to SeSAW [4] for structure-based function prediction (Fig. 6).

If your query contains intrinsically disordered domains (IDDs), they can be submitted to IDD Navigator [1-2]. IDD Navigator uses the composition of amino acids to query a database of similar IDDs. The Pfam domains and GO (Gene Ontology) terms associated with the stored IDDs are displayed along with the statistical significance of each match.
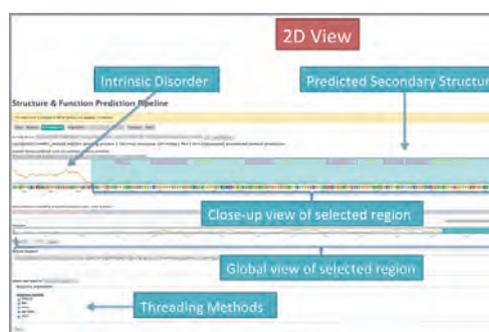
Fig.5: SFAS 2D View
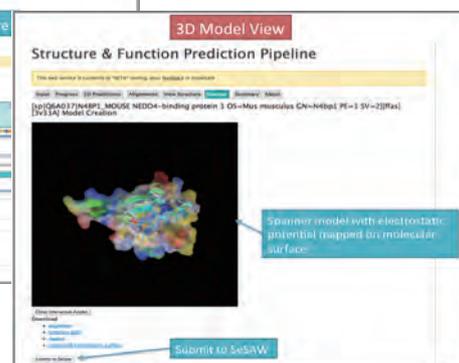
Fig.6: SFAS Spanner model view

[1] Teraguchi S., Patil A., Standley D. M. (2010) *BMC Bioinformatics* **11**, S7.
[2] Patil A., Teraguchi S., Dinh H., Nakai K., Standley D. M. (2011) *Pac. Symp. Biocomput.* **17**, 164-175.
[3] Lis M. *et al.* (2011) *Immunome Research* **7**.
[4] Standley D. M. *et al.* (2010) *Bioinformatics* **26**, 1258-1259.

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Public release of wwPDB/RDF

PDBj so far developed and provided RDF (Resource Description Framework)-formatted PDB data, which is standard in the Semantic Web, with the Ontology described in OWL translated from the PDBx schema [1]. Now, after slight revisions, the PDB/RDF has been provided from the wwPDB site, with the new URI of rdf.wwpdb.org. The top page of PDB/RDF has also changed to http://rdf.wwpdb.org/. Please use this URI from now on.

## Integrated NMR Analysis with virtual machine technology
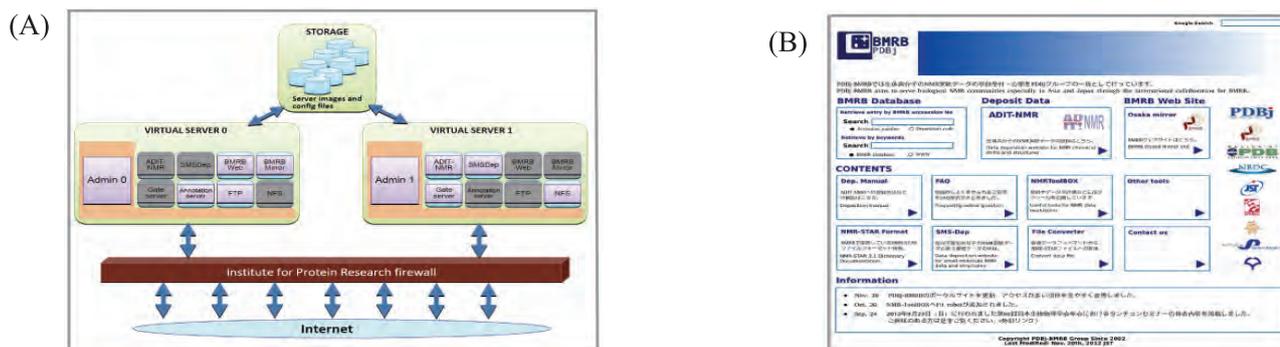
Fig.7: High robustness, power-saving and space-saving achieved on two PC-clusters by redundantly installed virtual servers derived from the eight physical servers used to work on PDBj-BMRB (A). Our renewed web-site to be opened shortly (B).

Kobayashi, N. et al., *J Biomol NMR* 53(4):311-320 (2012)
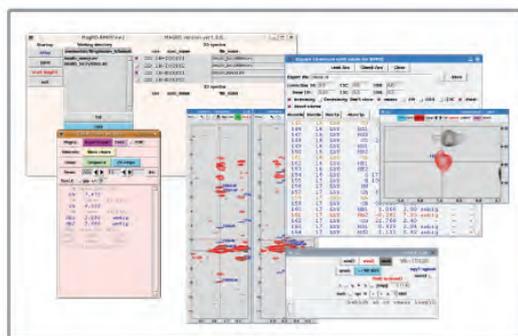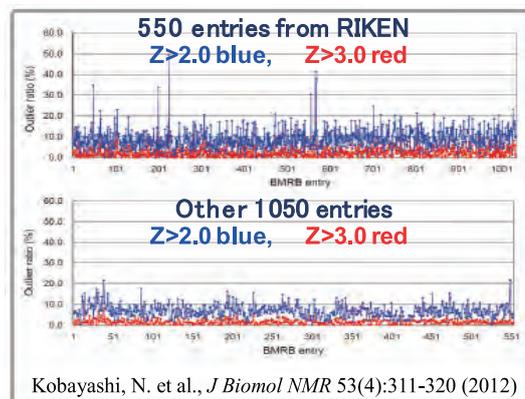
Fig.8: GUI tools to support the users for analysis and deposition of NMR experimental data implemented in MagRO-NMRView (C). Validation analysis performed by MagRO-validation for the 550 entries from RIKEN Structural Genomics Initiative (RSGI) (D-top) and 1050 entries from others (D-bottom). The entries from RIKEN show obviously as approximately twice good scores as the others.

PDBj-BMRB has been working with BMRB in Wisconsin and wwPDB, as a member of BMRB Scientific Advisory Board for the development of the NMR database, BioMagResBank (BMRB) , for discussing and exchanging ideas and opinions about management of deposition and annotation services. Recently, we have established a power-saving and space-saving server system with a high robustness for hardware failures, using virtual machine technology (Fig.7A). We are also planning to reopen our group web-site after being remodeled (Fig.7B). The new web-site will include the page to download our tools for analysis and deposition of NMR data (NMRToolBox) and renewed deposition manuals for BMRB. One of the tools, MagRO-NMRView, can facilitate analysis and deposition of NMR experimental data, demonstrating that the support of the program significantly increased quality of the data deposited to PDB and BMRB (Fig.8).

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