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Structural Life Science with Hybrid approach, and Roles of the wwPDB and the PDBj

Structural biology is to reveal atomic structures and shapes of proteins, nucleic acids, and their complexes based on the hierarchy in life science, and then to analyze the structure-function relationships. Because of a large gap between the analysis of cellular machineries and the above structural biology, multi-level studies beyond such hierarchic gaps have so far been very difficult. However, lots of new technologies such as super-resolution microscopy, cryo-electron microscopy (cryoEM), and combined light microscopy with EM, have been enabling to overcome the above gaps by hybridizing the methods of conventional structural biology and biochemistry: X-ray crystallography, Nuclear Magnetic Resonance (NMR), chemical cross-links, mass spectrometry, FRET, and computer simulation for dynamic molecular modeling.

In order to consider archiving those complex structures determined by the above hybrid, integrative approach, the wwPDB held a Task-Force meeting on October 6-7, 2014 at European Bioinformatics Institute (EBI), Hinxton, UK (Fig. 1).The Task-force members discussed about the experimental hybrid methods, description of the model data, and validation of the model qualities. Finally, they summarized recommendations to the wwPDB, who should take a leadership role in setting up federation.

Fig.1: Participants of the wwPDB Hybrid Methods Task-Force meeting on October 6-7, 2014 at EBI

From April 2014, the PDBj has updated its own database activity, supported by National Bioscience Database Center (NBDC), Japan Science and Technology Agency (JST) as the Database Integration Coordination Program. One of the PDBj missions in this Program is to search the similar shapes of the large molecular complexes from both PDB and EMDB archives (described later as “OMOKAGE” search), and to make the electrostatic molecular surface database (eF-site) for the large complexes (as in Fig. 2), in addition to visualize such large structures of cellular machineries.

In the near future, the hybrid, integrative methods surely become new trends of the life science, and all the members of the wwPDB including the PDBj will make their efforts to promote this scientific trend.

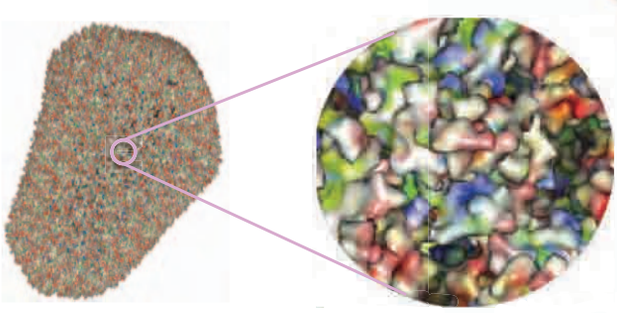


Fig.2: The electrostatic molecular surface of large structure, HIV-1 Capsid (3J3Q) composed of more than 2 million atoms (Blue: positive electrostatic potential, Red: negative electrostatic potential, and Yellow: hydrophobic surface).

News

The new wwPDB Deposition System

The wwPDB advisory committee meeting was held on 10 October 2014. At the meeting, the latest wwPDB deposition system was reviewed, and it was introduced that the numbers of deposited data have already been processed by the annotators at all the wwPDB sites. Because the system works well, the new wwPDB deposition system has been decided to be operated as the canonical deposition site for the X-ray crystal structures in 2015. Thus, from 2015, X-ray crystal structures are requested to be submitted using the wwPDB Deposition Tool (http://deposit.wwpdb.org/deposition). Deposition tools for NMR and 3DEM are being developed by the wwPDB, and will work in the near future.

Retire ADIT for Accepting Crystal Structures

As a result of this successful release, RCSB-PDB and PDBj will only accept depositions of structures determined from X-ray crystallographic experiments from the wwPDB Deposition Tool beginning January 27, 2015. At this time, the legacy ADIT deposition system will no longer accept new submissions of crystal structures. In-progress ADIT depositions of X-ray crystallographic structures will be able to access their deposition sessions until July 19, 2015.

ADIT will continue to accept depositions from other experimental methods. Deposition tools for NMR and 3DEM are being developed by the wwPDB.

Features of the new system include use of the PDBx/mmCIF data format, which produces more uniform data; the ability to replace data files pre- and post-deposition; enhanced communication; improved annotation; and geometric and experimental data checking based on recommendations from expert task forces. Detailed information and video tutorials are available.

Details;
http://pdbdep.protein.osaka-u.ac.jp/adit/ja/system_info_j.html

Video Tutrials;
http://pdbdep.protein.osaka-u.ac.jp/adit/ja/system_tutorial_j.html

PDBj Mine2 and its relational database

The backend relational database (RDB) of PDBj's general search system "PDBj Mine" (http://pdbj.org/mine) has been completely redesigned and now is released as PDBj Mine2 RDB. In this version, each PDBx/mmCIF category (http://mmcif.wwpdb.org/) corresponds to a table in PDBj Mine2 RDB. The "brief_summary" table is also available as in the previous version. Table definitions can be found at http://pdbj.org/mine-rdb-docs. These changes make it easier to write complex SQL queries that execute efficiently. Examples of various SQL queries can be found at http://pdbj.org/help/mine2-sql; these will help you construct your own queries. Along with other services, a REST API for SQL queries is also available (see http://pdbj.org/help/rest-interface). Furthermore, you can download and install the entire PDBj Mine2 RDB on your local system (PostgreSQL 9.3). Weekly updates as well as the entire dump file can be found at our FTP site (ftp://ftp.pdbj.org/mine2/) and a detailed instruction can be found at http://pdbj.org/help/mine2-rdb-local-install.

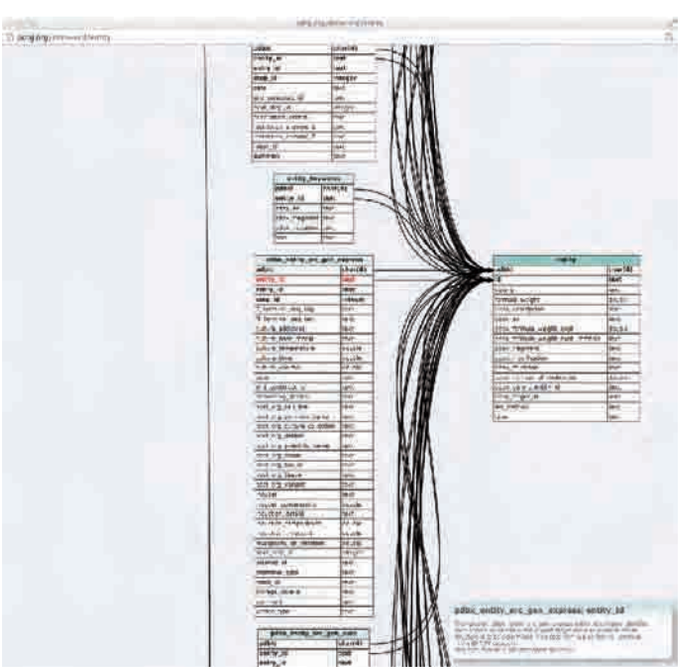


Fig.3: PDB diagram

Molmil: a new molecular viewer for the web

PDBj has developed a new molecular viewer by the name of molmil. Molmil runs directly within a modern web browser without the need of plugins such as Java or Flash. Furthermore, with its advanced shading engine it can produce smooth, realistic looking images. Together with an image exporter it allows users to produce high quality, high resolution images which can e.g. be used for publications. Finally, molmil also scales up so that it can display the largest structures available within the PDB.

In recent years mobile device such as tablets and smartphones have become more popular with the general population, but also within the scientific community. One of the characteristics of these mobile devices is that their web browsers generally do not have support for plugins. PDBj's previously developed molecular viewer jV requires Java and is as such not usable on mobile systems. Furthermore, due to ongoing endeavors by Oracle (the company developing Java) to improve the security of Java, the functionality of applets are increasingly becoming more limited. Web browser developers also have noticed the security issues of Java and have started blocking Java by default.

Improvements to web browsers in the last decade have however made it possible to use many advanced technologies which previously required a plugin. One such advanced technology is WebGL. WebGL allows a browser to draw a GPU accelerated 3D scene via a JavaScript API. For molmil, WebGL is the core technology for which without it, molmil could not exist.

Molmil has been integrated into many services PDBj provides; on the Mine PDB entry pages the Asymmetric Unit and when available the Biological Unit structures can be viewed using molmil. Also, the electron density map using the edmap service can be viewed using molmil when available. Our new Chemie service (which contains the chemical component entries part of the PDB) also has a molmil canvas directly implemented on the entry page. Other services which integrate molmil are Sequence Navigator & Structure Navigator (for the superimposed structures) and Promode Elastic (for the displacement vectors and motion animations). In the near future eF-site will also be upgraded with a molmil viewer.

There is also a standalone version of molmil available. Although it still requires the web browser, it doesn't load any structure or polygon data automatically when the page loads. Users can use it to load their own structures from their local hard drive. Molmil currently supports PDBx/mmCIF, PDBML and PDB flat files. Molmil also supports a new JSON based format developed by PDBj based on the PDBx/mmCIF format for optimized performance which is used when transferring data from the PDBj server to the user. Finally, molmil also has support for PDBj's polygon format (XML) which can be used to load arbitrary polygon data.

Molmil is available for desktops, laptops, tablets and smartphones given that both the browser and the display drivers are new enough. For more information on supported device, please take a look at the molmil help page: http://pdbj.org/help/molmil

Fig.4: Molmil for Mobile-type tablets

Omokage search – search by "shapes"

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

Imagine a biomolecule, which has a quite similar size and shape to the one you are interested in, while the structure elements or building blocks are distinct. If such the molecule were exists, are you interested in its functions and properties? For example, the complex of elongation factor-Tu and transfer RNA (protein-RNA complex) has the similar shape to the elongation factor G (single polypeptide). Both bind to the same site of the ribosome.

By Omokage search (Fig.5), a service we recently started, you may find such the structure data with "accidental resemblance". Ignoring the building elements and detailed structures, and comparing just the overall shapes, it searches EMDB and PDB for the structure data with similar shapes. Although Omokage search has such the unique aspect as a structure search tools, the original motivation was to make a structure-based search for EMDB, using fast comparison system designed for low-resolution electron microscopy (EM) data.

By Omokage search, EM users can easily confirm that whether their EM structures under the refinement process are enough similar to the appropriate structures in the databanks. Recently, EM structure papers published in high-impact journals are increasing. Even for the users not interested in EM methods, information about EM studies about the similar structures to the molecules of their interest may be useful.

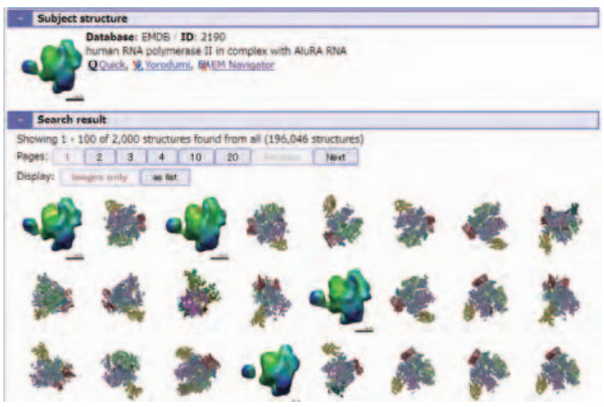


Fig.5: Result of Omoakge search

For the search, in addition to a structure data stored in EMDB or PDB, users can use an original structure data (an atomic model or 3D density map) as a search query by uploading the data to the server. A pseudo atomic model such as a SAXS bead model can also be used if it is in PDB format. In the result of page of search using structures in databanks, the links to corresponding gimfit page appear, so that users can see the similarity of structures within an interactive viewer showing the superimposed view (Fig.6).

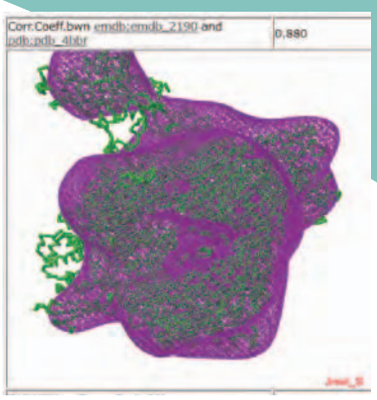


Fig.6: Superimposed view by gimift

PDBj-BMRB

Release of tool with new function to support fully automated analysis of NMR data

PDBj-BMRB group has developed new function implemented in MagRO-NMRView to support fully automated analysis of NMR data in combination with external programs FLYA and CYANA.

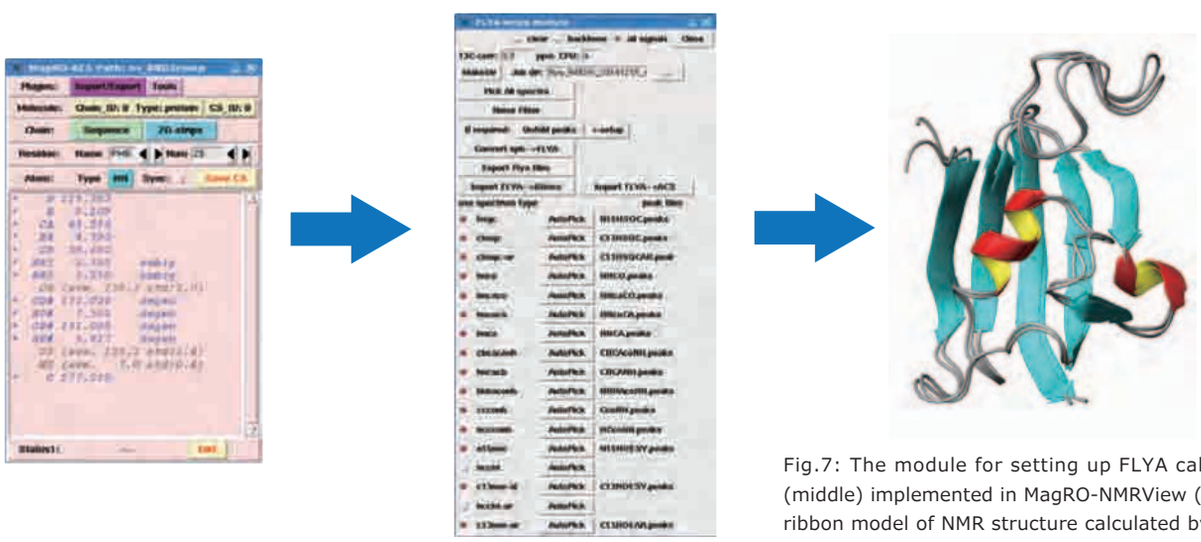


Fig.7: The module for setting up FLYA calculation (middle) implemented in MagRO-NMRView (left) and ribbon model of NMR structure calculated by CYANA

Release of tool for automatically extracting ordered regions in NMR structure ensemble

PDBj-BMRB group has developed and released a program tool named fit_robot which can automatically identify and extract ordered regions in an NMR structure ensemble. (Kobayashi, N. J. Biomol. NMR 2014).

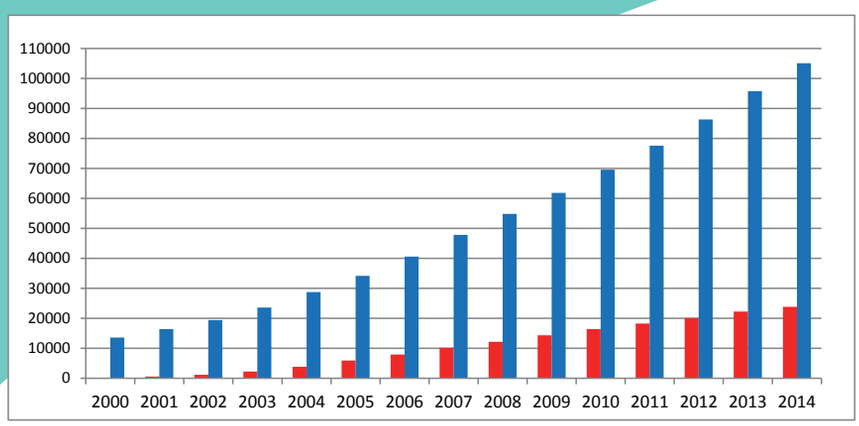
Conversion and publication of BMRB entries in XML and RDF formats

PDBj-BMRB group has developed tools for conversion of BMRB entries into data in XML and RDF formats and published them from the PDBj-BMRB web-site. The converted XML and RDF files are machine-readable and compatible with the NMR-START dictionary

which describes the data structure of BMRB database. The data with the standard semantic web technology will facilitate data exchange and knowledge discovery across diverse information resources.

Data Growth

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



*105,097, as of December 17, 2014

Event Report

Activities done for introducing PDBj and our newly developed web services.

Osaka University ICHO festival -Exbition for Protein Structure by 3D viewer
May 3, 2014, Institute for Protein Reseach

The 4th Asia Pacific Protein Association (APPA) Conference
- Poster, talks May 17-20, 2014, Jeju, Korea

The 12th Japan-Korea-China Bioinformatics Training Course
June 17-20, 2014, Jeju, Korea

Luncheon Seminar at 14th Annual Meeting of the Protein Science Society of Japan
JUNE 27, 2014, Yokohama, Japan

JST-NBDC Workshop for Database “AJACS AWA”
August 20, 2014, Tokushima, Japan

Luncheon Seminar at 52th Annual Meeting of the Biophysical Society of Japan September 27, 2014, Sapporo, Japan

PDBj & Plattform for Drug Dicovery, Informatics and Structural Life Science Joint Wokshop for Database October 1, 2014, Sendai, Japan

Luncheon Seminar at the 3rd Joint Conference on Informatics in Biology, Medicine and Pharmacrology
October 3, 2014, Sendai, Japan

Luncheon Seminar at the Annual Meeting 2014 of Crystallographic Society of Japan
November 3, 2014, Tokyo, Japan

Exbition Booth and Presentation at 37th Annual Meeting of the Molecular Biology Society of Japan
November 25-27, 2014, Yokohama, Japan

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

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