PDBj
Protein Data Bank Japan

http://www.pdbj.org/

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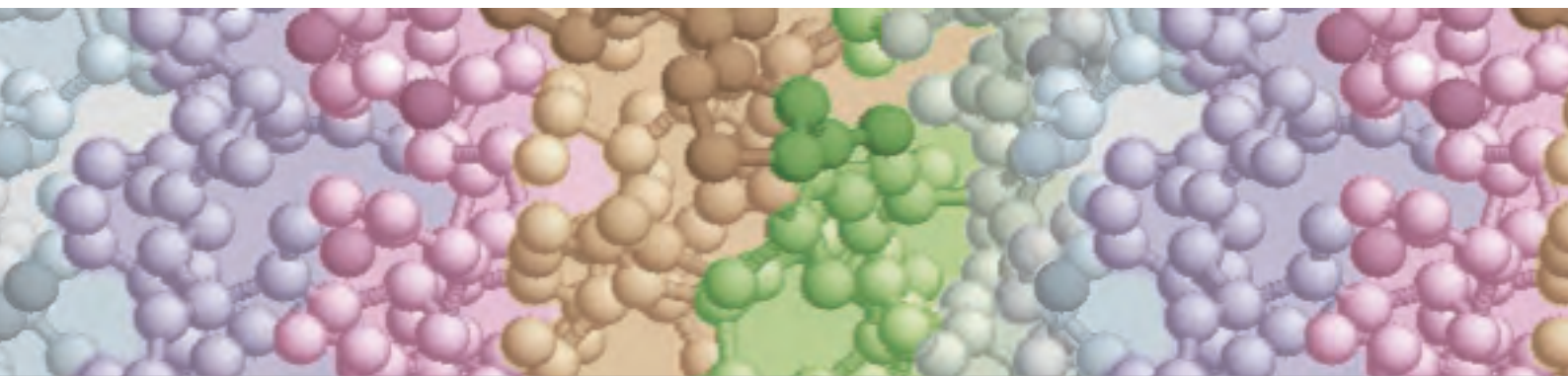
News

From December 2010, NMR assigned chemical shift becomes a mandatory requirement for a PDB deposition of every structure determined by NMR

On December 6th, 2010, as recommended by the wwPDB Advisory Board, assigned NMR chemical shift data is planned to be required in addition to restraints and NMR-determined atomic coordinates for a complete PDB deposition. Further, the atom nomenclature included in the assigned chemical shift file must be consistent with the atom nomenclature used in the atomic coordinate file, according to the IUPAC standard for standard residues. A new ADIT-NMR deposition system will be deployed at BMRB and PDBj-BMRB. To be able to carry out the atom nomenclature validation of the chemical shift file against that in the atomic coordinate file correctly, the assigned chemical shift data must be provided in the NMR-STAR v3.1 format. The STARch web service available at BMRB (http://bmrb.protein.osaka-u.ac.jp/software/starch/) can be used to convert assigned chemical shift data files in a variety of formats to the NMR-STAR v3.1 format. The ADIT-NMR system will attempt to convert non-IUPAC atom nomenclature for standard amino acids and nucleic acids found in both the uploaded coordinate and chemical shift file to the IUPAC standard. The atom nomenclature for non-standard amino acid and nucleotide residues found in the PDB Ligand Expo dictionary must conform to the Ligand Expo standard. The atom nomenclature of the coordinate file for non-standard residues not found in this dictionary must be consistent with that in the chemical shift file.

Small Molecular Structure Deposition (SMSDep) is now available at PDBj-BMRB

SMSDep site was established at PDBj-BMRB on August 23rd, 2010. This will become the unique SMSDep deposition site in the world. The SMS database is released by BMRB, and it is operated by the collaboration of BMRB and PDBj. SMSDep accepts atomic coordinates of a small molecule of biological interest determined by NMR together with constraints and chemical shifts. The small molecules are those that fall outside the scope of the PDB. The use of IUPAC atom nomenclature for standard amino acid and nucleic acid residues is strongly encouraged for both coordinates and NMR chemical shift tables. During annotation, non-IUPAC atom nomenclature will be converted to the IUPAC standard. If this is not carried out, the depositor will be required to provide a proper atom nomenclature mapping. The deposition process is basically the same as the new ADIT-NMR. The atom nomenclature for non-standard amino acid and nucleotide residues found in the PDB Ligand Expo dictionary must conform to the Ligand Expo standard. The atom nomenclature of the coordinate file for non-standard residues not found in this dictionary should be consistent with that in the chemical shift file. For the time being, only standard molecules and molecules with non-standard residues present in the PDB Ligand Expo dictionary will be fully validated. Validation and annotation are performed at PDBj and PDBj-BMRB.

Ichou Festival

The annual university festival, known as Ichousai, was held at Osaka University on April 30th and May 1st to welcome new students to the university, and a great opportunity to strengthen friendship and ties among the local community. We introduced our activities and the eProtS database, which is described further in this issue.
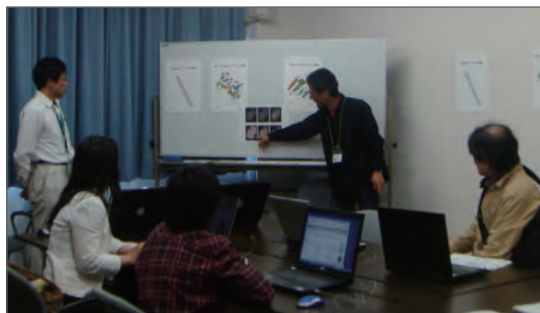
A snapshot of Ichou Festival.

The 10th Annual Meeting of the Protein Science Society of Japan

The 10th Annual Meeting of the Protein Science Society of Japan was held from June 16th to 18th, 2010 at the Sapporo Convention Center . We introduced our activities and services, and the BMRB database.

Life Science Database Workshop at Nagoya University

The life Science Database Workshop was held at Nagoya University on August 9th -10th in cooperation with DDBJ and DBLCS (Database Center for Life Science).

The 48th Annual Meeting of the Biophysical Society of Japan

The 48th Annual Meeting of the Biophysical Society of Japan was held from September 20th to 22nd, 2010 at Tohoku University, Kawauchi Campus. We introduced our activities and services at the Luncheon-seminar on 20th, and had the early-morning workshops on 21st-22nd from 8-9am.

InCoB2010 at Waseda University

InCoB2010 (The 9th International Conference on Bioinformatics) was held from September 26th to 28th at Waseda University, International Conference Center in collaborating with Chem-Bio Informatics Society of Japan and International Immunomics Society. We exhibited the booth during the conference.

Snapshots of the workshops. From left to right: the 10th PSSJ in Sapporo, the workshop at Nagoya University, the BSJ at Tohoku University and the InCoB2010 at Waseda University.

Data Growth

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

■ Processed structures by PDBj ■ Total available structures
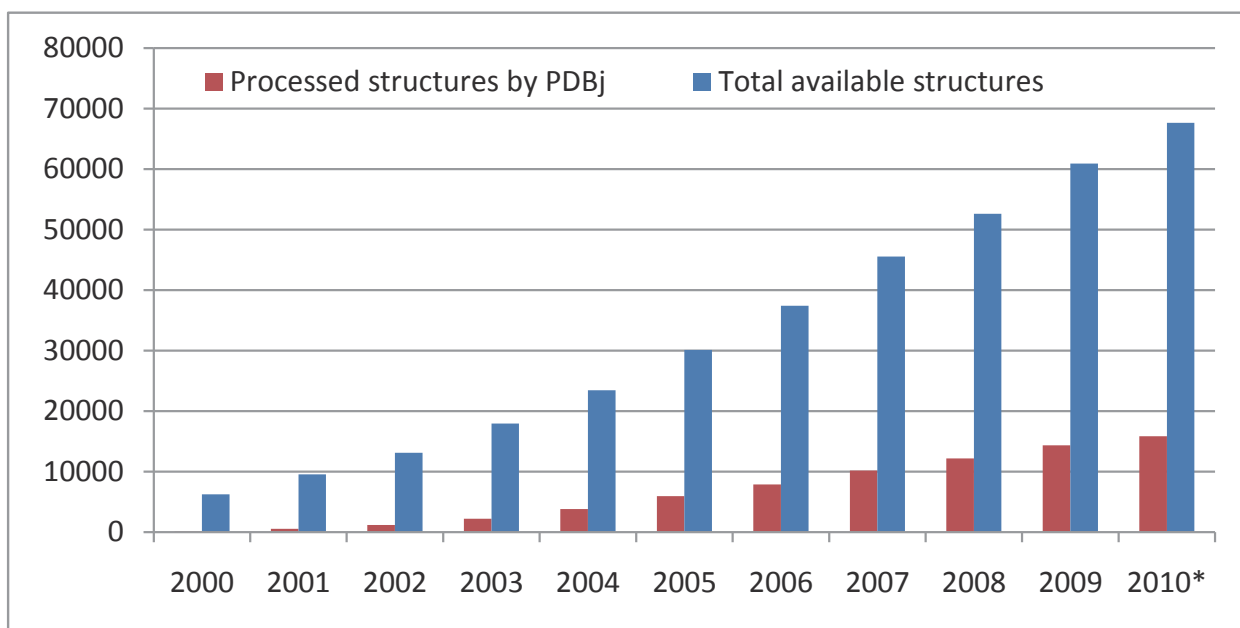
* Last updated : October 6, 2010

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Services

GIRAF

GIRAF(http://www.pdbj.org/giraf/) is a structure comparison and search service for interacting interfaces at atomic level. In its new version, one can now compare not only interfaces for protein-small molecule interfaces but also protein-protein and protein-DNA/RNA interfaces. Here, an ``interaction interface'' is defined as a set of atoms in a subunit that are within 5 Angstroms from a ligand (small molecules, DNA/RNA and proteins). The user can execute a search either by inputting a PDB ID or by uploading a PDB flat file (chain ID's can be also

The GIRAF frontpage.

specified). Search results are displayed as a list of matching entries, and for each entry, there is a more detailed result page with molecular graphics displayed using jV (PDBj's molecular graphics software). The database for interaction interfaces are updated every week to match the latest PDB, and contains all the known interfaces (except those for water molecules). As of September, 2010, more than 520,000 interfaces are stored. Due to the technique called ``geometric indexing,'' GIRAF can efficiently search this rather large database in a reasonable amount of time. Furthermore, it also produces atomic alignments of similar interfaces, enabling the user to closely examine the similarities at atomic resolution. Even when proteins are totally different with respect to their amino acid sequences and overall folds, their interaction interfaces may be similar, especially for mononucleotide- and ion-binding sites. Thus, GIRAF may be a useful option when you want to infer the functions of newly solved structures with unknown function. The search algorithm and its applications are in the following references.

【Reference】

1. Geometric similarities of protein-protein interfaces at atomic resolution are only observed within homologous families: An exhaustive structural classification study. Kinjo AR, Nakamura H. *Journal of Molecular Biology*, **399**:526-540 (2010).
2. Comprehensive structural classification of ligand binding motifs in proteins. Kinjo AR, Nakamura H. *Structure*, **17**:234-246 (2009).
3. Similarity search for local protein structures at atomic resolution by exploiting a database management system. Kinjo AR, Nakamura H. *BIOPHYSICS*, **3**:75-84 (2007).
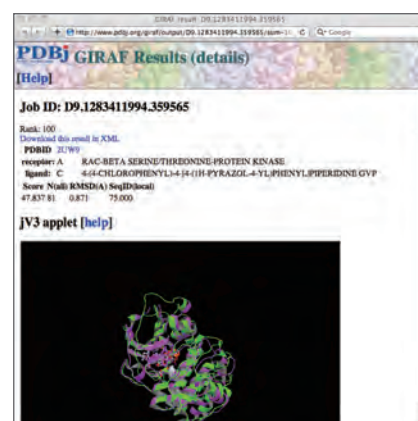
Examples of the GIRAF.

EMDB map data have been remediated

Many map data of EM Databank (EMDB, databank for 3D electron microscopy: http://www.pdbe.org/emdb/) have been remediated. The map data express 3D density distribution of the structure. As well as the density value of each point, it consists of geometry information of the map, such as the size and angle of the axes, and the numbers of points along the axes. Although the geometry information is very important to represent the structure precisely, it is not easy to make correct data for some reasons during the conversion procedure of the map data. By the efforts of EMDB staffs with the help of PDBj members, the geometry information in many data have been corrected. Now, many maps are in the same coordinate system as the fitted atomic models.
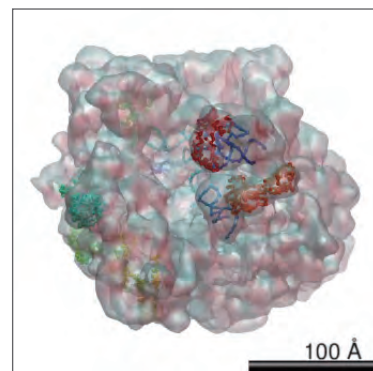
Superimposition of a remediated map data (EMDB-1003) with an atomic model (PDB-1eg0).

New features in EM Navigator

EM Navigator, a website to browse 3D electron microscopy data, has been developed so that even beginners and non-specialists can view the 3D structures easily and quickly. Recently, we have improved the two services. One is a new structure viewer page named "Yorodumi", which is a Japanese coinage, meaning "Tens of thousands of views". Although Yorodumi was first developed to visualize complex EM structures interactively, it now becomes available for most of the PDB and EMDB data. Users can easily view biological assembly structures, specific components in multi-subunit models, ligand binding sites, 3D EM maps, and so on. Yorodumi Gallery (Figure, right) in the top page of EM Navigator （http://www.pdbj.org/emnavi/viewtop.php) would be useful for tutorial. The other is an improvement for the movie interface. Now, the frame positions of the movies are shifted by positioning and moving the mouse pointer, so that the movies become more interactive and attractive than before. There are also some other improvements for specialists. Visit the EM Navigator (http://www.pdbj.org/emnavi) to see them!

An example of the Yorodumi Gallery.

jV3.8

jV3(http://www.pdbj.org/jv/), first released in 2004, is a molecular graphics program for display of proteins and nucleic acids, which can be used as an applet or as a stand-alone program. A new version, 3.8, released July 2010, provides increased functionality and enhanced stability.

jV3.8 supports the following three features: (1) GUI-based atom selectivity within a given molecule while displaying several molecules simultaneously; (2) the "displayatom" command, which permits easy switching between display/nondisplay on an atomic unit basis; and (3) the "File/save/PNG (JPEG)" command permits use of the save command while the program is used in applet mode.

Furthermore, we have improved the jV Wiki page making it easily accessible via the "Help" page (requires installation of Java 1.6 or higher), repaired various bugs, and enhanced overall usability within current Operating System environments.

Existing Users are encouraged to try jV3.8 and provide PDBj with any appropriate feedback. New Users are always welcome.
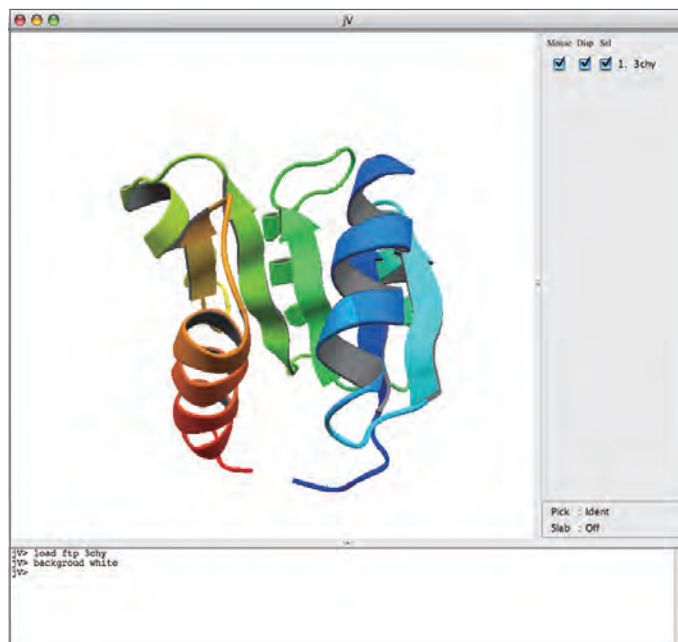
A display example of the jV3.8.

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