PDBj：Protein Data Bank Japan
（日本蛋白質構造データバンク）

Modifications to the Protein Data Bank: A new PDB format, Data Deposition, and Validation Report

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The Protein Data Bank Japan (PDBj, http://pdbj.org) is a member of the worldwide Protein Data Bank (wwPDB, http://wwpdb.org/) and accepts and processes the deposited data of experimentally determined macromolecular structures. While maintaining the archive in collaboration with other wwPDB partners, PDBj also provides a wide range of services and tools for analyzing structures and functions of proteins, which are summarized in this article. The wwPDB has recently decided to change its traditional "PDB format" in a plain text style to the "PDBx/mmCIF format, because of very many limitations in the "PDB format", such as limited chain and atom numbers, no bond order or chirality for ligands. We will discuss what are the differences, and how we are going to move to use the new format and its derived formats, PDBML and PDB/RDF, which are considered to be useful for data integration. Other important news from wwPDB is an opening of new annotation system for data deposition. This new annotation system enables workload balancing of data centers, increased productivity and better quality assurance of ligand chemistry and polymer sequences. We will also discuss about the validation report that summarizes quality of the deposited X-ray data and overview of the residue-based structural quality for every polymer. It will be used for reviewing papers describing macromolecular structures.

Browsing, searching, and compaing 3D electron microscopy data.

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Structure data derived by 3D electron microscopy (3DEM) deposited on PDB and EM Data Bank (EMDB) are increasing. We have been provided services for the 3DEM data. *EM Navigator* is a data explorer 3DEM data in both databanks. *Yorodumi* is interactive 3D structure viewer running on PCs and some mobile devices. While it is designed to see complex structures such as 3DEM data, all the PDB data and chemical component data also can be viewed. Recently, we start a new service, Omokage search, which is low-resolution shape similarity search system. Users can find structure data having similar shapes to users query structure from both of EMDB and PDB. Atomic models, 3D density maps, and SAXS bead models can be applied as a search query. Found 3DEM structure pair sharing shapes can be fitted by *gmfit*, and viewed interactively within web browsers. In the seminar, recent changes of PDB/EMDB format related to 3DEM in addition to our services will be introduced.

Tools for highly automated NMR analysis and applications using database

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Owing to the development of NMR analysis, highly automated methods have been available for NMR signal assignments and structure determination. The database for structure and experimental data has been growing so fast significantly raising the possibility to find homologues for the target macromolecule in the database. Nowadays we can apply homology modeling to NMR analysis.

We have recently developed a stand-alone system to expedite the tasks of NMR data analysis. The system is composed of a number of modules including graphical user interface (GUI) modules integrated by MagRO-Core and external programs such as a program for fully automated NOE assignments and structure determination (CYANA) and fully automated NMR signal assignments (FLYA). The modules for setting up FLYA and CYANA calculations are including fully automated peak picking, noise filtering and conversion of file format. Using the modules, the user can easily prepare peak lists for a wide variety of NMR spectra. For the calculations of FLYA and CYANA, the modules for importing the calculation results into the MagRO system support user to readily correct and assign remaining NMR signals. In the lecture, the procedure for analysis of the samples showing very broad signals will be shown, demonstrating that successful NMR signal assignments and structure determination can be performed using the structure generated by homology modeling.

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