

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

Activities of PDBj and wwPDB: A new PDB format, Data Deposition,
Validation, and Data Integration

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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”. 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 latest facilities of data deposition and validation will also be introduced.

The new PDBj web Interface: Customizable, Modern and User-friendly

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The new PDBj web interface was launched in May 2013 and now several months have passed. The new web interface offers a powerful search function, tightly integrated services, a customizable, modern and unified design, which also provides better responsiveness. All features and services familiar to users in the previous website (legacy) are still present in the new interface, but they have been redesigned and integrated into a single unified design. During the past couple of months we have made several modifications and improvements to the web interface. We have also developed a new version of the Mine RDB (Relational Data Base), which we will also introduce. During this talk we will introduce the new features and will give a demonstration on how the PDBj web interface can be used. As time passes, more functionality will be added. Upon user's requests, new features can also be added. Please contact us to suggest a feature to be included: <http://pdbj.org/contact>.

PDBj-BMRB: Publishing NMR Spectroscopy Derived Data of BioMagResBank in Structured Data Formats, XML and RDF

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The PDBj-BMRB (bmrdep.protein.osaka-u.ac.jp) at Osaka University operates a BioMagResBank (BMRB) site, which accepts data depositions and carries out data processing and annotation in close collaboration with the BMRB at the University of Wisconsin-Madison (www.bmrwisc.edu).

The BMRB is a repository for experimental and derived data gathered from nuclear magnetic resonance (NMR) spectroscopic studies of biological molecules. The NMR-STAR data format has been used in the ADIT-NMR deposition system, entry validation systems and the BMRB relational database for 15 years.

To enhance the interoperability of the BMRB archival data in addition to the NMR-STAR format, the PDBj-BMRB began to provide the data in standard structured data formats, which are an Extensible Markup Language (XML) and a Resource Description Framework (RDF). Collected data files of the formats are named BMRB/XML and BMRB/RDF, respectively.

We will discuss differences between the formats and introduce new publishing services (bmrpub.protein.osaka-u.ac.jp) for the BMRB/XML and BMRB/RDF with short examples.