Abstract

この文書では、高分子や生物分子の立体構造情報をより精度よく捉えるために、Protein Data Bank (PDB)を活用した研究が進められている。PDBは、国際的に認められたデータベースであるため、その情報の正確さと信頼性が高く、科学的な研究に不可欠である。

Protein Data Bank Japan (http://pdbj.org/)

Since 2001, PDBJ has been managed at Institute for Protein Research, Osaka University as a member of the wwPDB, to curate, edit and process the deposited data for and open, public, and single author of the PDB. The PDB archive contains more than 120,000 entries:

- "Data-in" activity, common in all the wwPDB members with high quality control. For the purpose, data deposition, validation system, versioning system, and new format are developed.
- "Data-out" services, common archive as the ftp site and the characteristic services by each wwPDB member.

Data in at PDBj and wwPDB

By now PDBj curates data and processes about a Quarter of the deposited data, mainly from Asian and Oceania regions.

PDBj Services

- Data-out from PDBj
- Molmil: Molecular Viewer based on WebGL developed by PDBj
- The SIFTS Data are integrated into PDBj Mine and wwPDB/RDF.

Database Integration

- wwPDB/RDF format for Semantic Web
- Integration to NBDC RDF-portal

Integration of PDB data with other databases through SIFTS (Structure integration with function, taxonomy and sequence)


PDBj Services

- Protein Molecular Surface DB
- Integration of PDB data with other databases through SIFTS (Structure integration with function, taxonomy and sequence)

Characteristic Data-out at PDBj

- Annotation of Protein Function from Molecular Surface Similarity
- PDBj-BMRB staff

Validation Report with experimental data

- PDB Deposits & Annotations
- Yearly deposited entries to wwPDB
- Collection of ORCID IDs (http://orcid.org/)

Large Structures in PDB

- As of December 2014, large structures are no longer split into multiple PDB entries but are released as single PDBx/mmCIF and PDBML files.
- By December 2018, all large structures have been released as single PDBx/mmCIF and PDBML files.
- Each wwPDB member provides tools to view large structures.

The SIFTS Data are integrated into PDBj Mine and wwPDB/RDF.

Omokage search: Search for similar SHAPES in PDB, EMDB and SASDB

Query: human RNA polymerase II with RNA (EMDB: 2190)