

Luncheon Seminar at the 54th Annual Meeting of Biophysical Society of Japan

November 25 (Fri), 11:45 ~ 12:35, Room 201 (C)

1. New issues in the wwPDB and the PDBj

wwPDB と PDB における新しい話題について

Haruki Nakamura, Institute for Protein Research, Osaka University

The PDBj (PDB Japan, <http://pd bj.org/>) is the representative archive of macromolecular structural data by X-ray crystallography, NMR and cryo-EM, processing the deposited data from researchers in Asian and Middle-east regions, as one of the four members of the wwPDB (worldwide PDB, <http://wwpdb.org/>). In order to promote the recent "Data Science", wwPDB now starts several new policies: (i) Usage of ORCID (Open Researcher and Contributor ID: <http://orcid.org/>) as the standard, (ii) Retiring the flat PDB format, (iii) Making the validation report more informative for NMR and cryo-EM data, (iv) Introduction of a versioning system, and (v) Change of the current 4-characters PDBID. Those issues will be introduced at the Luncheon Seminar.

2. Electron microscopy data in PDB and EMDB - deposition and browsing

EMDB と PDB における電子顕微鏡データ – 登録と閲覧

Hirofumi Suzuki, Institute for Protein Research, Osaka University

By recent innovations in electron microscopic (EM) methods, the number of EM structures in databanks is rapidly increasing. Atomic-model and density-map data by EM are separately stored in PDB and EM data bank (EMDB), respectively. While this separation is required for consistent management of the databanks, it may cause some intricacies in deposition and browsing the EM structure data. Therefore, we, wwPDB provide the new unified deposition system, OneDep. "One" of OneDep carries two meanings, one for the world, and one for the three structure databanks, BMRB, EMDB, and PDB. And also, we, PDBj renewed EM structure data explorer, EM Navigator. Now, it has renewed user interface unified with the structure viewer, Yorodumi and the shape similarity search, Omokage search. In the seminar I will introduce how to use and what you can get by these new systems.

3. New generation of NMR analysis assisted by Deep Learning and highly sophisticated Web-tools developed by PDBj-BMRB

PDBj-BMRB により開発された深層学習により支援された次世代 NMR 解析と高度化された Web ツール

Naohiro Kobayashi, Institute for Protein Research, Osaka University

NMR is a very unique and useful technique to analyze structure, dynamics and interaction with ligand of biomolecules in an atomic resolution easily and quickly. One of the largest burden on the NMR analysis would be identification and assigning very few signals among a huge number of noises and artifacts. Several programs are available to automatically assign the NMR signals, however none of them can start from NMR signal identification. Although NMR signal identification in multi-dimensional NMR spectra has been known to be a key job, many NMR scientists still prefer to spend a lot of time for preparing NMR signal tables manually. We have developed new generation of program MagRO which can discriminate weak but important NMR signals with huge number of artifacts and noises assisted by image recognition technology of Deep Neural Networks. We are going to demonstrate that our program has finally got "eyesight" like a human to enable highly automated, correct and fast calculation for sequence specific backbone signal assignments of protein.

We also will show our new web-tool that we have developed recently and released. The web-tool allows users easily and intuitively to search for a wide variety of information related to the studies on biomolecules: free keyword and sequence search to provide rich information such as NMR data (BMRB), structure coordinates (PDB), homologues and functions (UniProt), interactors (IntAct). The new NMR data page is designed to represent detail of the NMR parameters such as chemical shifts and dynamics data by highly sophisticated graphical interface as user can visually inspect interested domain region easily and straightforwardly.