



Protein Data Bank Japan

**Platform for Drug Discovery, Informatics,
and Structural Life Science**

Luncheon Seminar at the 53rd Annual Meeting of Biophysical Society of Japan

September 13 (Sun), 11:50-12:40, Room I (Lecture Room B)

Rapid advancement of high-resolution cryo-EM intrudes a database of atomic coordinates.

急速な高分解能クライオ電子顕微鏡の進歩による原子座標データベースの増加

Kenji Iwasaki, Institute for Protein Research, Osaka University

Almost every week the near-atomic resolution structures of various proteins determined by single-particle reconstruction (SPR) cryo-EM are reported in high profile journals, corresponding with a dramatic increase in the deposition of atomic coordinates into the PDB or EMDB. This revolution has been caused by the development of direct electron detection cameras. The rapid development of cryo-EM will be introduced in this seminar, along with a method developed in our laboratory: the hybrid approach, which combines EM, computer simulation, and crystal structures.

New deposition system and a validation tool of Protein Data Bank

Protein Data Bank の新しい登録システムと構造評価ツール

Atsushi Nakagawa, Institute for Protein Research, Osaka University

Because of recent advances of structure determination techniques, such as X-ray crystallography, NMR, cryo-EM etc, number of protein structures determined is dramatically increased. Furthermore, huge macromolecular complexes have been solved at atomic resolution. In the middle of 70s, when Protein Data Bank started to archive the atomic coordinates of proteins, only several tens of structures were deposited. The legacy PDB format has limited capabilities, since it is based on the techniques of computer and X-ray crystallography at that time. For example, number of chains is defined as one-byte capital character and number of residues is limited to 999. Large biological macromolecular assemblies, for example ribosome, exceeded these limitations. PDB decided to extend the PDB format to a new format, named PDBx/mmCIF, with much more capabilities. The PDBx/mmCIF is an extension of the legacy format, but it is more flexible. In addition to the new format, the new deposition system, which includes a validation tool, is now working in all PDB deposition sites since last January. All X-ray crystal structure must be deposited via the new deposition system and quality of the data can be assured with this new deposition system.

Introduction to Structural Life Science Data Cloud

構造生命科学データクラウドの紹介

Akira R. Kinjo, Institute for Protein Research, Osaka University

While protein structures provide detailed information about their molecular functions, it is often necessary to integrate such information in a broader context in order to understand the biological functions. In the Platform for Drug Discovery, Informatics, and Structural Life Science, we have been developing the VaPRoS system that amalgamates a wide range of information such as genomes, gene expression, protein structures, protein complexes, and more. In this seminar, I will introduce some of the basic functionalities of the VaPRoS system for the end user.

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<http://pd bj.org/>

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