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場所: 臨海副都心センター別館 8 階コラボレーションコーナー
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タイトル
Next Generation Protein 3D Structure Analysis: Rapid Global/Local Surface Comparison, Docking and Low-Resolution Data

概要
The protein 3D structure contains crucial information for understanding biological systems and also essential for protein design and rational drug design. Protein structural bioinformatics is an active research area that develops and applies computational techniques for analyzing protein structures.
Protein structural bioinformatics is facing new challenges raised from needs of analyzing an increasing number of solved protein structures, low-resolution structural data from electron microscopy or tomography, predicted structures, as well as structures of unknown function. To enable efficient global and local protein structure analysis, our group has been using a protein surface representation with the 3D Zernike descriptors (3DZD). The 3DZD are series expansion of a three dimensional mathematical function that can represent a 3D object in a rotation and translational invariant fashion. In this talk we will discuss several applications of the protein surface representation. First, we will introduce on our method named 3D-SURFER, for real-time searching of global protein structures, which can be in low-resolution. Next, application to local pocket matching for binding ligand prediction will be discussed.
Finally, we applied 3DZD for shape-based protein-protein docking. Our new docking algorithm, LZerD (local 3D Zernike descriptor-based Docking algorithm), uses the 3DZD for capturing local shape complementarity of interacting protein surfaces. LZerD has been further extended recently for multiple protein docking and also for fitting multiple protein structures into a density map of electron microscopy.

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