

Development of Structural Genomics Tool Based on Protein-Ligand Binding Structures

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Understanding the protein-ligand interaction is very important in post-genomics biological science because many proteins require small molecular ligands or cofactors such as ATP or NAD. The first step for understanding protein-ligand interaction would be to analyze all the known protein-ligand complex structures in the Protein Data Bank (PDB, <http://www.rcsb.org>). Recently, we have developed a novel Web-based bioinformatics tool, called PDB-Ligand (<http://www.idrtech.com/PDB-Ligand/>), for the visual and interactive clustering of all the known protein-ligand complexes in PDB. (1)

PDB-Ligand is a database and a tool that allows one to browse, classify, superimpose and visualize these protein-ligand binding structures. Currently, there are about 5390 types of small molecular ligands and more than 130,000 protein-ligand complex structures, experimentally determined as a complex with protein or DNA. One novel feature of PDB-Ligand is that it allows an interactive clustering of ligand-binding structures based on user-specific clustering criteria with flexible combinations of atoms or residues at the ligand-binding sites. PDB-Ligand, when using with other related ligand-binding structure analysis tools, will be a good resource for better understanding of ligand-binding structures, which may be critically important in many new drug discovery applications.

Reference

- (1) Jae-Min Shin & Do-Ho Cho (2005), PDB-Ligand: a ligand database based on PDB for the automated and customized classification of ligand binding structures, *Nucleic Acids Research*, 33, D238-D241.