MS12-P06

Bringing together functional annotations related to structure

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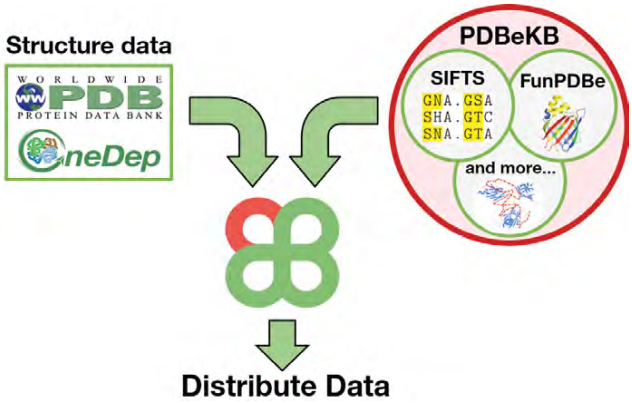
In order to understand macromolecular structures archived in the Protein Data Bank (PDB), it is essential to take into consideration the biological context of these molecules. Multiple specialised resources each provide one or more aspects of the biological context, but it takes significant effort to collect and compare all the information that may be relevant to a specific structure.

PDBe-KB (Protein Data Bank in Europe - Knowledge Base) is a new community driven resource under development by PDBe, which will provide functional annotations for structural data that can be used by the scientific community to answer biological questions. PDBe-KB is a collaborative effort between PDBe and a diverse group of biological resources and structural bioinformatics research teams. This new resource will consolidate older services, such as SIFTS, which focuses on providing seamless mappings between PDB entries and other databases, and data from multiple data enrichment projects. These include the FunPDBe project, which aims to collect and distribute highly enriched, valuable annotations that create a comprehensive biological context for structural models, effectively bringing structure to biology.



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MS12-P07

Conservation and Variability in Hydrogen Bonding in Proteins

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Hydrogen bonds are an essential part of the structure and function of proteins, defining the secondary structure and the overall fold of the protein as well as being important components of the active sites of enzymes. However, despite the widespread belief that proteins are evolved to sustain a single, folded structure, there is significant, empirically demonstrable variability in the hydrogen bonding pattern of proteins, even within sets of identical protein structures in which there is little overall structural variation. Hydrogen bond variability has been recently clearly demonstrated in a set of structures of a single protein bound to a homologous series of ligands[1]. However, neither the extent of this variability, nor its function has been widely otherwise remarked upon in the current literature. We catalogue the variability of hydrogen bonding patterns in all currently publically known protein structures present in the Protein Data Bank[2]. We use a geometric definition of hydrogen bonding in proteins to focus on the kind of data available from x-ray structures of proteins. We compared the hydrogen bonding pattern between all instances of identical or nearly identical proteins (≥ 90 % sequence identity) which have been deposited at least 10 times in the PDB (n ~ 6500) and used this redundancy to measure the inherent variability in a given hydrogen bond. This geometric definition will allow treatment of both strong (e.g. OH-O, NH-O) and weak/non-traditional (e.g. CH-O, NH-π, OH/NH-S, etc.) protein hydrogen bonds. Identification and characterization of this variability will help to understand the role of this variability in protein structure and also aid in future protein engineering and design efforts.

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