Oral presentation

T Leveraging PDBe, PDBe-KB, and AlphaFold Protein Structure Database for Enhanced Structural Biology

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The Protein Data Bank in Europe (PDBe) and the Protein Data Bank in Europe Knowledge Base (PDBe-KB) are crucial in structural biology. As part of the Worldwide Protein Data Bank (wwPDB), PDBe archives and provides global access to 3D structural data of biological macromolecules. It offers robust tools for searching and retrieving structural information based on sequence, structure, function, and biological context. Advanced visualisation tools, like Mol*, allow users to explore and analyse macromolecular structures in 3D and understand spatial relationships within complexes.

PDBe-KB complements PDBe by integrating and standardising information from multiple sources, providing comprehensive data about macromolecular structures. It enhances the utility of the PDB with detailed annotations on functional, biological, and biochemical information, linked to experimental evidence and literature references. Interactive visualisation tools in PDBe-KB help users explore structural features and functional sites, while cross-references to related databases offer additional context, such as disease-related databases, biological functions, and biochemical pathways, to further enrich the data.

The AlphaFold Database, developed by DeepMind and EMBL-EBI, provides high-quality predicted structures for over 214 million proteins. Key features include confidence metrics such as per-residue confidence score (pLDDT) and Predicted Alignment Error (PAE), and interactive 3D visualisation tools, which facilitate detailed examination of protein structures.

Together, PDBe, PDBe-KB, and the AlphaFold Database enhance the accessibility, functionality, and collaborative potential of structural biology data. These platforms offer powerful tools for data retrieval, analysis, and visualisation, along with detailed annotations and educational resources. We support advanced research in molecular biology, biochemistry, pharmacology, and bioinformatics. By helping scientists understand molecular mechanisms, design new drugs, and explore macromolecular structures and functions, they facilitate research and discovery. Additionally, they provide tutorials, articles, and guides to assist researchers, educators, and students in effectively utilising structural data.