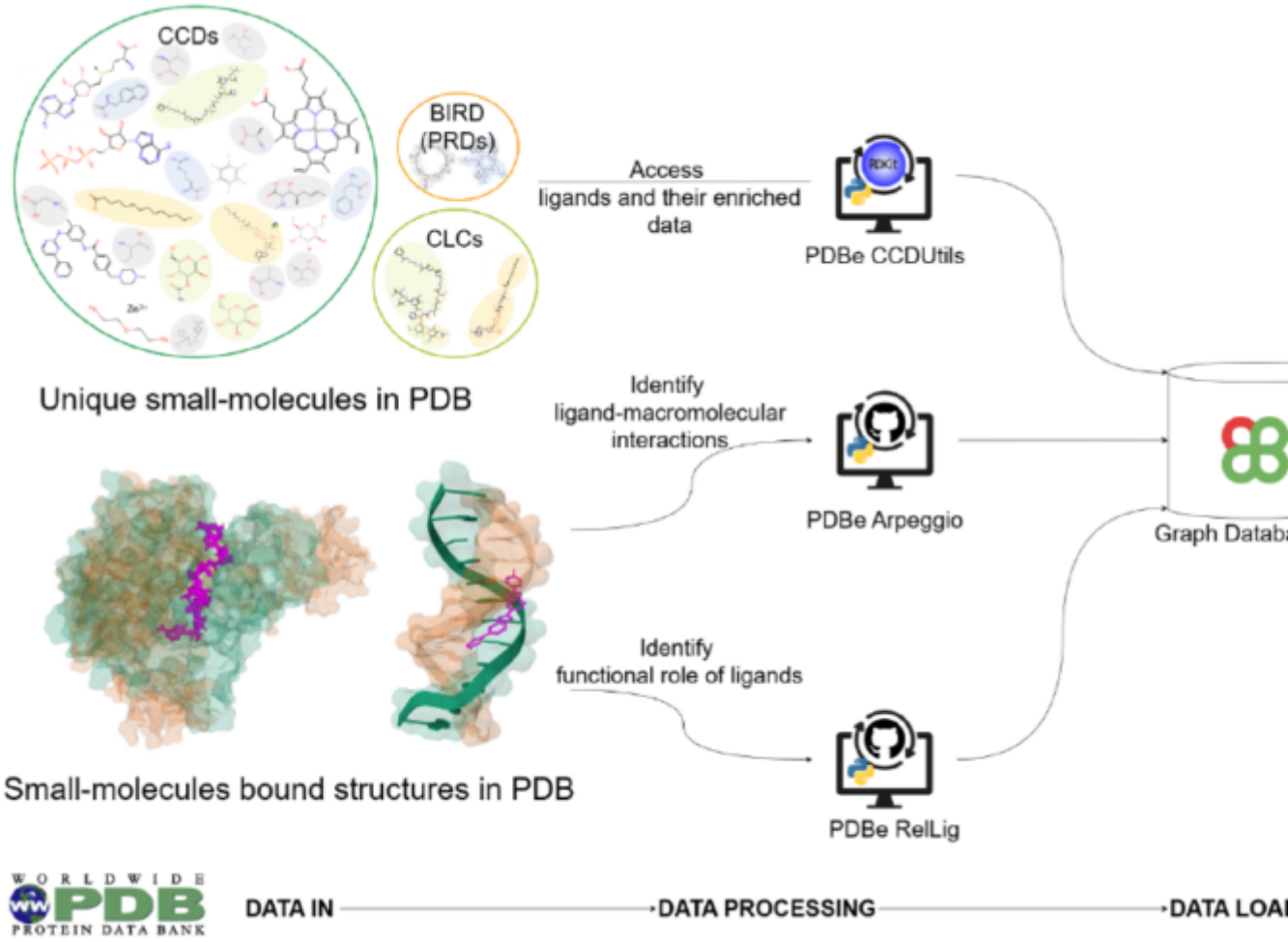
PDBe tools for an in-depth analysis of small molecules in the Protein Data Bank

Description

The Protein Data Bank (PDB) is the worldâ??s premier repository of experimentally determined 3D structures of biological macromolecules and their complexes with ligands, proteins, and nucleic acids. The PDB contains over 47,000 unique small molecules bound to macromolecules. Despite the large amount of data available, the complexity of the small molecule data in the PDB requires specialized tools for practical analysis and visualization. PDBe has developed several tools, including PDBe CCDUtils (https://github.com/PDBeurope/ccdutils) for accessing and enriching ligand data, PDBe Arpeggio (https://github.com/PDBeurope/arpeggio) for analyzing interactions between ligands and macromolecules, and PDBe RelLig (https://github.com/PDBeurope/rellig) for identifying the functional roles of ligands (such as reactants, cofactors, or drug-like molecules) within protein-ligand complexes. In addition, the enhanced ligand annotations and data generated by these tools are presented in a comprehensive view on the new PDBe-KB ligand pages, providing a holistic view of small molecules and enabling the establishment of their biological context (example page for Imatinib: https://wwwdev.ebi.ac.uk/pdbe-srv/pdbechem/chemicalCompound/show/STI).



By improving the standardization of ligand identification, adding rich annotations, and providing advanced visualization capabilities, these tools help researchers navigate the complexities of small molecules and their roles in biological systems, facilitating a mechanistic understanding of biological functions. Ongoing enhancements to these resources are designed to help the scientific community gain valuable insights into ligands and their applications in various fields, including drug discovery, molecular biology, systems biology, structural biology, and pharmacology.

Category

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