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Computational Approaches to Accelerate Drug Discovery

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Abstract

Protein-ligand interactions are fundamental to numerous biological processes. These interactions are indispensable for cellular communication, metabolic pathways, immune responses, and numerous other vital functions. A comprehensive understanding of protein-ligand interactions is crucial for drug discovery and development. This study examines the intricate mechanisms underlying these interactions, with a focus on the role of non-covalent forces such as hydrogen bonding, electrostatic interactions, van der Waals forces, and hydrophobic effects. By elucidating the molecular determinants of binding affinity and specificity, various drug design strategies have been explored to target specific proteins implicated in disease pathogenesis. This involves understanding the intricate interplay of non-covalent interactions, including hydrogen bonding, electrostatic interactions, van der Waals forces, and hydrophobic effects, that govern the formation of protein-ligand complexes. Computational approaches, such as molecular docking and dynamics simulations, have become indispensable tools in drug discovery, enabling the identification of novel protein targets, pharmacophore mapping, molecular docking, virtual screening of lead compounds, prediction of bioactivity, simulation of protein-ligand complex dynamics, affinity prediction, and the design of optimized ligands. These techniques enable researchers to virtually screen vast chemical libraries, identify potential drug candidates, and refine their structures to enhance binding affinity and selectivity. By simulating the dynamic behavior of protein-ligand complexes, these computational methods provide valuable insights into the molecular mechanisms underlying drug action, ultimately accelerating the drug discovery process.[1][2]

Key words: Protein-ligand interaction, molecular docking, dynamics simulations, drug discovery.

References

[1] Kataria A, Srivastava A, Singh DD, et al. Systematic computational strategies for identifying protein targets and lead discovery. RSC Medicinal Chemistry, 15: 2254–2269, 2024.

[2] Decherchi S, Cavalli A. Thermodynamics and Kinetics of Drug-Target Binding by Molecular

Simulation. Chemical Reviews, 120: 12788–12833, 2020.