International Journal of Chemical Sciences

Editorial | Vol 22 Iss 2

Molecular docking predicts the interaction between small molecules and biological targets for rational drug design

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Received: feb 04, 2024; **Accepted:** feb 18, 2024; **Published:** feb 27, 2024

Abstract

Molecular docking is a computational technique used to predict how small molecules, such as drug candidates, bind to biological targets like proteins and nucleic acids. By simulating binding orientations and estimating interaction energies, docking studies guide rational drug design and reduce the need for extensive experimental screening. This approach integrates chemistry, biology, and computer science to identify promising therapeutic compounds efficiently. This article discusses the principles, methodologies, and applications of molecular docking in modern medicinal and computational chemistry.

***Keywords:** Molecular docking, Drug design, Protein–ligand interaction, Binding affinity, Computational modeling, Structure–activity relationship, Virtual screening, Chemical biology, Therapeutic discovery, Bioinformatics*

Introduction

Molecular docking is a powerful computational approach that predicts how a small molecule fits into the binding site of a biological macromolecule, typically a protein, to form a stable complex [1]. This method is fundamental to rational drug design because biological activity often depends on how well a drug candidate interacts with its target at the molecular level. By simulating these interactions, chemists can prioritize compounds with the highest likelihood of therapeutic effectiveness. The docking process involves two main components: predicting the orientation of the ligand within the binding site and estimating the binding affinity through scoring functions. These scoring functions evaluate hydrogen bonding, hydrophobic interactions, electrostatic forces, and steric compatibility between the ligand and the target [2]. The best docking pose corresponds to the most energetically favorable configuration. Structural data obtained from techniques such as X-ray crystallography and NMR spectroscopy provide detailed models of biological targets, which serve as the foundation for docking simulations. Advances in computational power allow rapid screening of thousands of compounds through virtual screening, significantly accelerating the drug discovery process [3]. Molecular docking is closely linked to the

Citation: Amina Rahbek. Molecular docking predicts the interaction between small molecules and biological targets for rational drug design. Int J Chem Sci. 22(2):443.

concept of structure–activity relationship, where changes in ligand structure influence binding efficiency and biological response. By analyzing docking results, chemists can modify functional groups to enhance selectivity and reduce side effects. This iterative process between modeling and synthesis optimizes potential drug candidates. Docking studies are also applied beyond pharmaceuticals, including enzyme engineering, pesticide design, and understanding biochemical pathways. Integration with molecular dynamics simulations further refines predictions by accounting for flexibility in both the ligand and the target [4]. The accuracy of docking depends on reliable algorithms, accurate structural data, and appropriate scoring methods. Continuous improvements in software and computational methods enhance predictive reliability and expand the scope of docking applications [5].

Conclusion

Molecular docking provides an efficient method for predicting interactions between small molecules and biological targets, supporting rational drug design and virtual screening. By combining computational modeling with chemical insight, docking accelerates the discovery and optimization of therapeutic compounds. Ongoing advancements in algorithms and structural analysis will further strengthen its role in chemical and biomedical research.

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