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Molecular Docking: A Modern Approach for Drug Discovery

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ABSTRACT

Molecular docking is an essential computational technique widely used in drug discovery to predict the interaction between the small molecules and their protein targets. This poster presents an examination of molecular docking, including its historical development and current relevance in pharmaceutical research and life sciences. It outlines the core principles of molecular docking, differentiating between rigid and flexible molecular docking methods. It also highlights the role of molecular docking in identifying and validating drug targets, supported by case studies demonstrating successful applications. Additionally, it covers the identification and optimization of lead compounds through virtual screening (v.s.) processes. Recent advancements in docking methodologies, such as the integration of machine learning and artificial intelligence. It illustrates the application of molecular docking in various therapeutic areas, including oncology, infectious diseases, and neurological disorders, with relevant examples. The challenges faced in molecular docking, such as accuracy, computational demands, and the need for experimental validation, are also discussed. Thus, molecular docking is a powerful computational tool that plays a critical role in drug discovery and development. The role of molecular docking is expanding beyond traditional drug discovery to include personalized medicine, quantum computing, and applications in environmental and agricultural sciences. It helps in target identification and validation, lead compound identification, and lead optimization. Recent advances, such as the integration of AI and machine learning and coupling with other computational methods, have significantly enhanced its accuracy and efficiency.

Keywords: *Computational techniques, rigid & flexible molecular docking, validating drug target, artificial intelligence, machine learning*

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