Chapter 1
Molecular Docking and Its Applications in Nanotechnology

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ABSTRACT

This chapter explores the intersection of molecular docking and nanotechnology, highlighting how computational methods drive innovations at the nanoscale. The fundamental principles and algorithms of molecular docking are highlighted before moving on to its pivotal role in nanotechnology. The applications are diverse, from improving drug delivery systems through enhanced interactions between nanoparticles and drugs to guiding the precise design of nanomaterials through protein-nanomaterial interactions. The chapter includes case studies that provide real-world examples of molecular docking's applications. It also addresses challenges and offers a balanced perspective on integrating molecular docking in nanotechnology. The

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chapter explores future directions and emerging trends, envisioning advancements in docking algorithms and their potential impact on future nanotechnology innovations. In conclusion, the chapter outlines implications for nanotechnology advancements and encourages the exploration of molecular docking in nanotechnology.

INTRODUCTION

In drug discovery and design, molecular docking is a computer tool commonly used to predict the binding affinities and modes of small compounds, or ligands, to target proteins or receptors, (Abdelsattar, Dawoud, & Helal, 2021). Molecular docking (MD) helps to find promising drug candidates with therapeutic efficacy by modelling the atomic-level interaction between ligands and receptors, (Abo-zeid et al., 2020). The most energetically advantageous binding pose is found using algorithms that search the conformational space of the ligand and the receptor. Molecular docking has developed into an effective drug development method, helping clarify structure-activity correlations and optimize lead molecules, (Agarwal & Mehrotra, 2016). MD is widely used in drug discovery as it is a cost-effective and simplified computational method. The MD is widely applied to find new molecules from normal to rare diseases, (Agu et al., 2023). Apart from drug discovery, it is also used to assess the toxicity of drug candidates. Various studies have been conducted during the pandemic to select and discover therapeutically effective vaccines or drug molecules for treating COVID-19, (Akbarzadeh et al., 2022). Apart from drug discovery, MD is widely used in formulation development. It is pivotal in formulation development because it predicts how drug candidates interact with target proteins or receptors. It expedites drug discovery through virtual screening of compound libraries, identifying potential candidates for further study. Docking simulations also optimize formulations by assessing drug-excipient interactions and predicting stability. Crucially, it elucidates molecular interactions, guiding the design of drugs with enhanced efficacy and reduced side effects, (Anselmo & Mitragotri, 2019). Additionally, docking aids in predicting ADMET properties early, influencing drug development strategy and resource allocation. Overall, molecular docking integrates computational tools with biochemical insights, significantly advancing the efficiency and success of pharmaceutical formulation development. Integrating molecular docking with nanotechnology represents a promising frontier in scientific research, offering novel approaches for drug delivery, diagnostics, and therapeutic interventions, (Ayesha et al., 2023). There several studies have reported on the application of MD in formulation development. Yousuf et al. performed the MD on *Piper nigrum* seed extract-loaded emugel to check its anti-ageing activity with targeted proteins, (Bansal et al., 2021). Integrating molecular docking with nanotechnology

Benzoxazoles: Diverse Biological Activities and Therapeutic Potential

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