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AI-Assisted Virtual Screening and Molecular Docking for Rational Drug Discovery: A Systematic Review

Communication Info

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Abstract

The discovery of novel therapeutics is a time-consuming and capital-intensive process and costs over $2.6 billion per drug [1]. According to those limitations, the emergence of virtual screening (VS) and molecular docking were critical computational strategies to accelerate lead identification [2]. However, classical scoring functions suffer from limited accuracy [3].

The emergence of artificial intelligence (AI), specifically deep learning (DL), motivated by recent advances like AlphaFold [4], has revolutionized computer-aided drug design

This systematic review, conducted in accordance with the PRISMA 2020 guidelines [5], provides a comprehensive analysis of AI techniques in virtual screening. The review also highlights a critical gap in multi-target drug discovery strategies, which remain underrepresented despite their clinical importance for complex diseases.

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