Quantum-Inspired Molecular Docking for Drug Discovery Targeting Biochemical Pathways

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***Abstract*—Molecular docking is a central technique in drug discovery, enabling the prediction of interactions between small molecules and biological targets within complex biochemical pathways. However, classical docking algorithms often face limitations when navigating high-dimensional conformational spaces, accounting for protein flexibility, and identifying optimal binding configurations across large compound libraries. This study explores the application of quantum-inspired molecular docking frameworks as an alternative approach to address these challenges. By drawing on principles such as superposition-inspired parallel search, probabilistic state exploration, and optimization heuristics derived from quantum computing, quantum-inspired models aim to enhance docking accuracy and computational efficiency without requiring fully fault-tolerant quantum hardware. Through qualitative synthesis of research in computational chemistry, drug design, and quantum-inspired optimization, this paper examines how these methods can improve the identification of biologically relevant binding poses and pathway-specific targets. The analysis highlights potential advantages in modeling multi-target interactions, allosteric effects, and pathway-level drug responses. The findings suggest that quantum-inspired docking approaches offer a promising framework for accelerating early-stage drug discovery and for advancing precision medicine by enabling more robust exploration of biochemical interaction networks. Ultimately, this study positions quantum-inspired molecular docking as a scalable and forward-looking strategy for targeting complex biological systems.**

Drug discovery is an inherently complex and resource-intensive process, requiring the identification of molecular compounds capable of selectively interacting with biological targets involved in disease-related biochemical pathways [9]. Molecular docking has emerged as a foundational computational technique in this process, enabling researchers to predict ligand–protein interactions, estimate binding affinities, and prioritize candidate molecules for experimental validation [8]. Despite its widespread use, classical molecular docking faces persistent challenges related to computational scalability, conformational flexibility, and the accurate modeling of dynamic biological environments.

Biochemical pathways often involve networks of interacting proteins, enzymes, and regulatory molecules rather than isolated targets. Effective therapeutic intervention therefore requires a pathway-aware approach that accounts for multi-target interactions, feedback mechanisms, and allosteric

Digital Object Identifier 10.62802/ab9rd645

Date of publication 11 12 2025; date of current version 11 12 2025

