Quantum-Inspired Molecular Docking for Drug Discovery Targeting Biochemical Pathways

Duru Çakır
Uskudar American Academy

***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

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regulation [2]. Classical docking algorithms, which typically evaluate ligand–target pairs sequentially and rely on approximated scoring functions, struggle to fully capture this complexity. As compound libraries and structural databases continue to expand, the combinatorial explosion of possible molecular configurations further limits the efficiency of traditional methods [5].

Recent advances in quantum computing and quantum-inspired optimization offer a novel perspective on these challenges. While practical quantum computers remain limited, quantum-inspired algorithms adapt mathematical principles from quantum theory—such as parallel state exploration and probabilistic optimization—to run on classical hardware [7]. In the context of molecular docking, these approaches enable more efficient exploration of conformational landscapes, improved global optimization of binding poses, and enhanced handling of uncertainty in molecular interactions [1].

Quantum-inspired molecular docking reframes the docking problem as a high-dimensional optimization task in which multiple ligand conformations and binding sites can be evaluated simultaneously through probabilistic sampling strategies [3]. This allows for more effective navigation of rugged energy landscapes and reduces the likelihood of convergence to suboptimal local minima. Furthermore, these models can be extended to pathway-level analyses, supporting the identification of compounds that modulate entire biochemical networks rather than single molecular targets [6].

The integration of quantum-inspired docking methods holds particular promise for precision medicine and systems pharmacology, where understanding pathway interactions is critical for minimizing side effects and maximizing therapeutic efficacy. By enabling more comprehensive modeling of molecular interactions, these approaches can accelerate early-stage drug discovery and improve candidate selection prior to costly experimental trials [4].

This paper explores the theoretical foundations, methodological advantages, and application potential of quantum-inspired molecular docking for drug discovery targeting biochemical pathways. Through an interdisciplinary review of computational chemistry, optimization theory, and emerging quantum-inspired methods, the study argues that these approaches represent a significant step toward more efficient, scalable, and biologically informed drug discovery pipelines.

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