

Quantum Computing in Drug Discovery

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Abstract

Drug discovery is a computationally intensive, multistage pipeline encompassing target identification, molecular simulation, virtual screening, molecular docking, lead optimization, toxicity prediction, and experimental validation. Although classical computational tools have advanced the field, accurately modeling electronic structures and complex molecular interactions remains difficult due to the inherently quantum mechanical nature of subatomic physics. Quantum computing offers an alternative paradigm leveraging qubits, superposition, entanglement, and interference to overcome these limitations. This paper reviews the application of quantum computing across key drug discovery phases, including quantum chemistry, molecular dynamics, virtual screening, docking, quantum machine learning (QML), and generative molecular design. We discuss foundational algorithms and frameworks, such as the Variational Quantum Eigensolver (VQE), variational quantum circuits, quantum optimization, and hybrid quantum-classical workflows. Furthermore, we evaluate the critical constraints imposed by current Noisy Intermediate-Scale Quantum (NISQ) hardware—including high error rates, restricted qubit counts, fault-tolerant overhead, measurement costs, circuit depth limitations, and the challenge of proving quantum advantage over state-of-the-art classical baselines. Synthesis of current literature indicates that the most viable near-term trajectory is a hybrid architecture where quantum coprocessors target specific subproblems rather than an end-to-end quantum pipeline. Ultimately, the long-term impact of quantum computing on pharmaceutical discovery hinges on concurrent breakthroughs in fault-tolerant hardware, quantum algorithms, error correction, efficient data encoding, rigorous benchmarking, and seamless integration with existing computational chemistry and AI workflows.

Keywords: Quantum computing; drug discovery; quantum chemistry; molecular simulation

I. INTRODUCTION

The discovery of a new therapeutic molecule is a complex scientific and economic process. Researchers must identify a biological target, discover or design candidate molecules, evaluate their interactions with the target, optimize potency and selectivity, investigate pharmacokinetic and toxicological properties, and ultimately validate promising candidates experimentally. Computational drug discovery has become an important part of this process because it can reduce the number of compounds that must be synthesized and tested in the laboratory.

A central challenge is that molecular behavior is governed by quantum mechanics. The distribution and correlation of electrons determine chemical bonding, molecular geometry, charge distributions, reaction pathways, and many properties relevant to drug activity. Classical computers can approximate these effects using methods such as density functional theory, Hartree-Fock methods, coupled-cluster approaches, molecular mechanics, and molecular dynamics. However, the computational cost can become substantial as the size and complexity of a molecular system increase.

Quantum computing is therefore being investigated as a possible technology for selected computational bottlenecks in chemistry and drug design. A 2024 Nature Physics perspective emphasized both the promise of quantum chemical calculations and the substantial gap between present quantum hardware and the requirements of realistic pharmaceutical systems, which may involve thousands of atoms at finite temperature. (Santagati et al., 2024)

The purpose of this paper is to review the current research landscape, explain the major quantum-computing approaches relevant to drug discovery, identify promising applications, and critically examine the barriers that must be overcome before quantum computing can deliver reliable pharmaceutical value.

Objectives of the Study

- To explain the fundamental concepts of quantum computing relevant to drug discovery.
- To examine applications of quantum computing in molecular simulation, docking, virtual screening, molecular dynamics, and molecular design.
- To discuss important quantum algorithms and hybrid quantum-classical approaches.
- To investigate the role of quantum machine learning in drug discovery.
- To identify current technical, computational, and practical limitations.
- To evaluate future research directions and the conditions required for useful quantum advantage.



Fig.1. Role of quantum computing in Health science

II. RESEARCH METHODOLOGY

This paper uses a narrative literature-review methodology. Peer-reviewed research articles, review papers, and perspectives published by major scientific publishers and indexed biomedical literature databases are examined. Particular attention is given to recent work on quantum computing for drug design, quantum machine learning, molecular simulation, and prioritization of quantum use cases in pharmaceutical research. The review emphasizes evidence published from 2024 through 2026 while also incorporating foundational concepts needed to explain the algorithms.

The literature was analyzed according to five themes: (1) quantum chemistry and molecular simulation, (2) quantum algorithms, (3) drug-discovery applications, (4) quantum machine learning, and (5) hardware and algorithmic limitations. The analysis distinguishes demonstrated capabilities from prospective applications.

III. RESULT AND DISCUSSION

A. Fundamentals of Quantum Computing

1. Classical Bits and Qubits

A classical bit takes the value 0 or 1. A quantum bit, or qubit, is described by a quantum state that can be written as $|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$, where α and β are complex probability amplitudes satisfying $|\alpha|^2 + |\beta|^2 = 1$. This property is called superposition.

Quantum systems can also exhibit entanglement, in which the state of multiple qubits cannot be described independently. Quantum algorithms exploit superposition, entanglement, and interference to manipulate probability amplitudes. These

properties are particularly relevant to chemistry because electrons and molecular states are themselves quantum mechanical.

2. Quantum Chemistry

The electronic structure of a molecule can be described by the time-independent Schrödinger equation $H\Psi = E\Psi$, where H is the Hamiltonian, Ψ is the molecular wavefunction, and E is the corresponding energy. Solving this equation exactly for realistic molecules is generally infeasible on classical computers, so practical chemistry relies on approximations.

Quantum computers provide a natural representation for quantum states. In principle, a sufficiently capable fault-tolerant quantum computer could represent molecular electronic states and estimate quantities such as ground-state energies with methods designed for quantum hardware. This possibility is one of the main scientific motivations for quantum computing in chemistry and drug discovery.

B. Quantum Algorithms Relevant to Drug Discovery

1. Variational Quantum Eigensolver

The Variational Quantum Eigensolver (VQE) is a hybrid quantum-classical algorithm designed to estimate molecular ground-state energies. A parameterized quantum circuit prepares a trial state, the quantum processor measures the expectation value of the molecular Hamiltonian, and a classical optimizer updates the circuit parameters to minimize the estimated energy. The variational principle provides an upper bound to the ground-state energy for an appropriate trial state.

VQE is attractive for current noisy quantum processors because it can use relatively shallow circuits compared with some early fault-tolerant algorithms. However, practical performance is affected by circuit depth, noise, measurement overhead, ansatz design, optimizer behavior, and the number of measurements required. Recent drug-discovery literature identifies VQE and related quantum-chemistry algorithms as important research directions but not yet as replacements for mature classical chemistry software.

2. Quantum Approximate Optimization Algorithm

The Quantum Approximate Optimization Algorithm (QAOA) is a variational approach intended for combinatorial optimization. In drug discovery, optimization problems can occur in molecular selection, feature selection, conformational search, and other discrete decision problems. QAOA may therefore be relevant to selected optimization subproblems, although practical pharmaceutical advantage has not been established generally.

3. Quantum Machine Learning

Quantum machine learning (QML) combines machine-learning concepts with quantum circuits. A typical QML workflow includes classical data preprocessing, encoding of information into a quantum state, application of a parameterized quantum circuit, measurement, and classical post-processing. A 2025 Chemical Reviews article surveyed quantum neural networks, variational quantum circuits, data encoding, molecular property prediction, and molecular generation in drug discovery.

Potential QML applications include predicting molecular properties, estimating drug-target interactions, classifying compounds, ranking candidates, and generating molecules. However, QML models must be compared against strong classical machine-learning baselines, and practical issues such as data encoding and quantum measurement can reduce or eliminate theoretical advantages.

C. Applications in Drug Discovery

1. Molecular Simulation

Molecular simulation is one of the most scientifically compelling applications. Quantum methods could eventually improve the calculation of electronic structures, reaction energies, molecular geometries, and other properties relevant to ligand binding and chemical reactivity. The long-term objective is to model chemically relevant portions of drug-target systems at an accuracy and scale that are difficult to achieve classically.

2. Molecular Docking

Molecular docking predicts how a small molecule may fit into a protein binding site. Classical docking searches through ligand poses and evaluates them using scoring functions. Quantum computing may contribute to selected optimization or energy-evaluation stages of docking. Potential areas include pose optimization, flexible docking, and improved energy calculations. However, complete protein-ligand docking remains far beyond the capabilities of current quantum hardware.

3. Virtual Screening

Virtual screening reduces a large chemical library to a smaller set of candidates for experimental testing. Quantum approaches may be incorporated into candidate ranking, optimization, similarity analysis, or quantum-enhanced machine learning. A realistic near-term architecture is likely to use classical screening to reduce the chemical space and then apply quantum methods to selected high-value problems.

4. Molecular Dynamics

Molecular dynamics simulates the time-dependent behavior of molecules. In drug discovery, it can be used to study protein flexibility, ligand stability, conformational changes, and interactions. Quantum computing could eventually accelerate selected components of molecular-dynamics workflows or improve quantum-mechanical calculations embedded in multiscale simulations. Current research remains exploratory, particularly for large-scale sampling.

5. Molecular Property Prediction

Drug candidates must satisfy multiple chemical and biological constraints. Machine-learning models can predict properties such as solubility, toxicity, permeability, potency, and binding affinity. Quantum machine learning is being investigated as an alternative or complement to classical models. The strongest potential use is likely to be hybrid: classical models handle large datasets while quantum circuits are evaluated for selected representations or prediction tasks.

6. Hybrid Quantum-Classical Architecture

The most realistic near-term model is a hybrid quantum-classical workflow. Classical computers would perform data storage, preprocessing, conventional molecular docking, large-scale screening, machine learning, and validation. Quantum processors would be used selectively for electronic-structure calculations, optimization, or quantum-machine-learning components.

A representative workflow is: chemical library → classical preprocessing → classical screening → quantum chemistry or quantum optimization → classical ranking → molecular simulation → experimental validation. This architecture reflects the current limitations of quantum hardware while allowing researchers to investigate where quantum computation might provide measurable value.

7. Advantages and Potential Benefits

- Natural representation of quantum-mechanical molecular states.
- Potentially improved accuracy for selected electronic-structure problems.
- Potential acceleration of particular optimization problems.
- Possible integration with artificial intelligence and generative chemistry.
- Potential reduction of experimental search space through improved computational prediction.
- A pathway toward new computational approaches for chemistry that are difficult to reproduce efficiently using classical representations.

D. Challenges and Limitations

1. Noise and Decoherence

Current quantum processors are noisy. Interactions with the environment can destroy quantum information, and gate errors accumulate as circuits become deeper. This limits the size and accuracy of useful calculations.

2. Limited Qubit Resources

Realistic drug-target systems can involve thousands of atoms and many electronic degrees of freedom. Current devices cannot directly represent complete pharmaceutical-scale systems at the required accuracy.

3. Error Correction

Fault-tolerant quantum computing requires error-correcting codes and substantial physical-qubit overhead. Large-scale chemistry applications therefore depend on advances in hardware reliability, logical qubits, and error-correction efficiency.

4. Measurement Overhead

Variational quantum algorithms often require many repeated measurements to estimate expectation values. This sampling cost can become a major bottleneck.

5. Barren Plateaus and Optimization

Parameterized quantum circuits can suffer from optimization difficulties such as barren plateaus, where gradients become extremely small. This can make training variational quantum models difficult.

IV. CONCLUSION

Quantum computing represents a promising long-term technology for drug discovery because chemistry is fundamentally governed by quantum mechanics. Potential applications span quantum chemistry, molecular simulation, docking, virtual screening, molecular dynamics, quantum machine learning, and generative molecular design. VQE, QAOA, variational quantum circuits, and quantum neural networks provide important research directions.

At the same time, current quantum computers remain limited by noise, qubit counts, error-correction overhead, measurement costs, and optimization difficulties. The available evidence therefore supports a cautious conclusion: quantum computing is not yet a general replacement for classical computational chemistry, but it is a serious research direction for selected problems where future hardware may deliver measurable advantages. Hybrid quantum-classical workflows are the most credible near-term path. The decisive milestone will be demonstrated quantum advantage on realistic, scientifically meaningful drug-discovery tasks rather than performance on isolated toy problems.

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