JOURNAL OF PHARMA INSIGHTS AND RESEARCH ISSN NO. 3048-5428

REVIEW ARTICLE

Applications of Quantum Computing in Drug Development

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Publication history: Received on 7th April 2025; Revised on 3rd May 2025; Accepted on 4th May 2025

Article DOI: 10.69613/m089dd39

Abstract: Drug development remains a complex, time-intensive, and costly process, with high failure rates in clinical trials. The advent of quantum computing presents promising opportunities to transform pharmaceutical research and development through enhanced molecular simulations and structure-based drug design. Quantum computing uses quantum mechanical phenomena like superposition and entanglement to process complex molecular interactions more efficiently than classical computers. The integration of quantum computing with machine learning algorithms has enabled more accurate predictions of drug-target interactions and improved virtual screening of compound libraries. Applications include structure-based drug design, molecular docking, lead optimization, and drug repurposing. Notable progress has been made through collaborations between pharmaceutical companies and quantum computing firms, demonstrating practical implementations in drug discovery workflows. However, several challenges persist, including hardware limitations, algorithmic maturity, skilled workforce gaps, and regulatory considerations. The combination of quantum computing with classical computing and machine learning approaches offers a hybrid framework that maximizes the strengths of each technology. As quantum computing technology advances, it is positioned to significantly impact pharmaceutical research and development, potentially reducing development timelines and improving success rates in drug discovery. This review explains the principles, current applications, integration, and limitations of quantum computing in drug development.

Keywords: Quantum Computing; Drug Discovery; Molecular Simulations; Structure-Based Drug Design; Drug Repurposing.

1. Introduction

Drug discovery has evolved significantly since its origins in early human civilization, where treatments primarily relied on natural substances discovered through observation and experimentation [1]. The modern drug development process represents a complex series of stages requiring substantial investments in time and resources, often extending beyond a decade from initial discovery to market approval [2, 3]. A drug, defined as a foreign substance capable of altering biological processes for therapeutic purposes, can originate from either natural or synthetic sources [4]. The journey from concept to approved medication involves multiple phases, beginning with target identification and proceeding through compound screening, lead optimization, and extensive clinical trials [5].

The foundation of modern drug research emerged in the early 1900s, primarily within academic settings [6]. This initial phase typically focuses on identifying macromolecules, such as genes or proteins, or disrupted signaling pathways linked to specific disease conditions [7]. The identification of appropriate therapeutic targets presents significant challenges, as drug effectiveness depends on both specific activity at intended targets and potential interactions with unintended targets [8]. The traditional drug development pathway progresses through several stages: basic research, target identification, lead compound discovery, preclinical testing, clinical trials, regulatory review, and post-market surveillance [9]. Clinical trials, conducted in multiple phases, evaluate drug safety and efficacy in human subjects to determine optimal benefit-to-risk ratios [10]. Following successful trials, regulatory agencies assess the data to determine market approval. Post-approval pharmacovigilance studies continue to monitor long-term safety and effectiveness [11].

Current challenges in traditional drug development include low success rates, with over 90% of candidates failing to achieve regulatory approval [12]. The process demands extensive resources and time - for instance, the development of an effective malaria treatment required 35 years [13]. Additionally, the necessity for large-scale human trials poses inherent risks to participants, particularly in early development stages [14].

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Recent technological advances offer potential solutions to these challenges. The integration of artificial intelligence, biotechnology, and quantum mechanics into drug discovery processes has opened new avenues for pharmaceutical research [15]. Quantum computing, in particular, presents opportunities to optimize drug development processes through enhanced computational capabilities [16].

2. Quantum Computing in Life Sciences

2.1. History

The foundation of quantum computing was laid by Richard Feynman's 1981 lecture on quantum mechanical computers [17]. Feynman proposed that quantum systems could be effectively simulated using computers based on quantum mechanical principles, laying the groundwork for modern quantum computing [18]. This interdisciplinary field integrates principles from physics, computer technology, and mathematics to enhance computational capabilities through quantum mechanical phenomena [19].

Table 1. Comparison of Classical and Quantum Computing Techniques in Drug Discovery

Parameter	Classical Computing	Quantum Computing
Molecular Modeling Capacity	Limited to small/medium molecules	Can handle complex molecular systems
Simulation Speed	Hours to days for complex molecules	Potential for exponential speedup
Resource Requirements	High memory for large molecules	Requires fewer qubits for complex calculations
Accuracy in Electronic Structure	Approximations often necessary	More accurate quantum mechanical calculations
Scaling with System Size	Exponential scaling	Polynomial scaling potential

Quantum mechanics studies matter and light behavior at molecular levels, enabling scientists to determine atomic and molecular properties [20]. The distinctive power of quantum computing stems from two fundamental quantum phenomena: superposition and entanglement [21]. Unlike classical computers that process information using bits (0 or 1), quantum computers utilize quantum bits or qubits, which can exist in multiple states simultaneously through superposition [22].

2.2. Molecular Modeling

The unique capabilities of quantum computers make them particularly valuable for simulating molecular interactions, a crucial aspect of drug discovery [23]. These systems can process complex molecular datasets simultaneously, offering advantages over classical computing methods in several areas:

2.2.1. Molecular Interaction Simulation

Quantum computers excel at simulating molecular dynamics and predicting interaction patterns between drug candidates and their targets [24]. This capability enables more accurate modeling of drug-protein interactions and better prediction of therapeutic outcomes [25]. The quantum approach accounts for subtle electronic interactions, van der Waals forces, and other quantum mechanical effects that play crucial roles in molecular binding. These simulations can capture transient states and intermediate configurations that are difficult to observe experimentally, providing insights into binding mechanisms and drug efficacy.

2.2.2. Optimization of Drug Properties

The enhanced computational power allows for precise prediction of drug candidate properties, helping researchers identify molecules with optimal therapeutic potential and minimal adverse effects [26]. This capability extends to understanding complex chemical reactions, including enzyme-catalyzed processes and protein folding mechanisms [27]. Quantum computing enables researchers to optimize multiple drug properties simultaneously, including solubility, permeability, stability, and binding affinity. The technology facilitates the exploration of vast chemical spaces, allowing for the identification of novel molecular structures with desired properties. Additionally, quantum computers can model the electronic structure of molecules with greater accuracy, leading to better predictions of chemical reactivity and physical properties.

2.2.3. Precision Medicine

Quantum computing facilitates the development of individualized therapeutic approaches by enabling accurate predictions of drug-patient interactions based on genetic profiles [28]. This capability supports the advancement of personalized medicine through more precise molecular modeling and interaction predictions [29]. The technology allows for the integration of multiple data types, including genomic, proteomic, and metabolomic information, to create comprehensive patient profiles. These profiles can be used to predict drug responses and potential side effects with greater accuracy. Quantum computers can analyze complex patterns in

patient data to identify subtle differences in drug responses among different population subgroups, leading to more targeted and effective therapeutic strategies. This method also enables the identification of biomarkers that can predict treatment outcomes and guide drug selection for individual patients.

3. Quantum Computing in Drug Development

3.1. Structure-Based Drug Design

Structure-based drug design (SBDD) represents a crucial application of quantum computing in pharmaceutical research. This approach utilizes three-dimensional structural information of biological targets to design highly specific binding molecules [30]. Quantum computing enhances SBDD through several mechanisms, revolutionizing traditional approaches to drug design and development. The integration of quantum mechanical principles allows for a more comprehensive understanding of molecular interactions at the atomic level, leading to more efficient and accurate drug design processes.

Table 2. Current Applications of Quantum Computing in Drug Development Stages

Development Stage	Quantum Computing Application	Current Status	Advantages
Target Identification	Protein folding simulation	Early implementation	Enhanced accuracy in structure prediction
Lead Discovery	Molecular docking	Proof of concept	Faster screening of compound libraries
Lead Optimization	Property prediction	Active development	Better prediction of drug properties
Clinical Trial Design	Patient stratification	Theoretical stage	Improved patient-drug matching
Drug Repurposing	Interaction modeling	Early implementation	Rapid screening of existing drugs

3.1.1. Accurate Molecular Docking

Quantum algorithms, particularly the Variational Quantum Eigensolver (VQE), provide more accurate simulations of electronic structures and molecular dynamics [31]. This enhanced accuracy leads to better predictions of binding affinities and reduces false positives in drug candidate screening [32]. The quantum approach accounts for subtle electronic effects and conformational changes that classical computing methods often oversimplify or ignore entirely. The VQE algorithm specifically excels in calculating ground-state energies of molecular systems, modeling electron correlation effects, predicting molecular geometry optimizations, and evaluating transition states in chemical reactions. These fundamental capabilities have transformed researchers' ability to understand protein-ligand interactions at unprecedented levels of detail. The improved understanding extends to the identification of previously unknown binding sites and the prediction of binding pose stability. Moreover, the quantum approach enables more accurate consideration of environmental factors, including water molecules and their role in binding interactions.

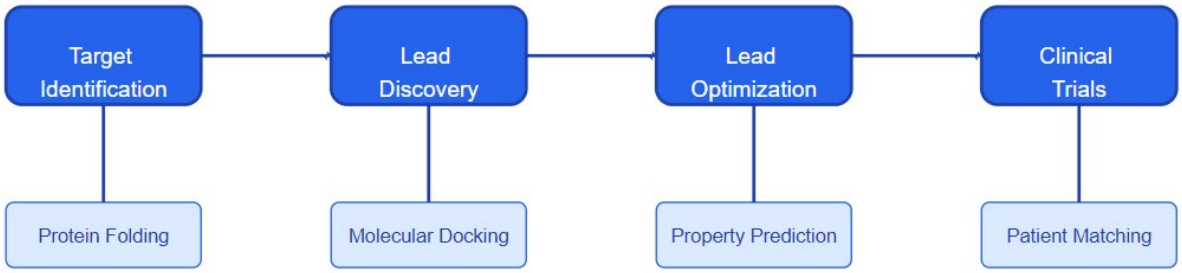

Figure 1. Quantum Computing in Drug Development

3.1.2. Improved Scoring Functions

Quantum computing enables more sophisticated scoring functions for evaluating drug-target interactions [33]. These advanced calculations incorporate quantum chemistry methods such as coupled-cluster theory and density functional theory (DFT), resulting in more reliable predictions of binding energies and molecular properties [34]. The enhanced scoring functions represent a significant advancement over classical methods through several key improvements.

In terms of energy evaluation, quantum computing methods provide more accurate treatment of electronic effects and better representation of hydrogen bonding. The approach offers improved modeling of van der Waals interactions and enhanced

consideration of polarization effects. The precise evaluation of entropic contributions has become more reliable, leading to more accurate predictions of molecular behavior in biological systems. The advanced property predictions enabled by quantum computing include better estimation of binding free energies and more accurate prediction of conformational changes. The improved evaluation of solvent effects and enhanced understanding of electronic structure contribute to more reliable calculations of physicochemical properties. These capabilities have significantly improved the accuracy of drug development predictions.

The implementation of quantum-enhanced scoring functions has resulted in reduced false positive rates in virtual screening and more efficient lead optimization processes. The improved prediction of drug-like properties and better ranking of potential drug candidates have streamlined the drug development pipeline. Additionally, more accurate estimation of binding kinetics has enhanced researchers' ability to predict drug efficacy. The integration of quantum mechanical principles in scoring functions has revolutionized hit identification and reduced the requirements for experimental validation. Researchers now have a better understanding of structure-activity relationships and improved ability to predict drug resistance mechanisms. The enhanced capabilities in designing multi-target drugs have opened new possibilities in therapeutic development. These improvements in molecular docking and scoring functions have created significant implications for drug development. The process has seen accelerated drug discovery timelines and reduced costs in experimental validation. Higher success rates in clinical trials have been observed, along with more efficient lead optimization processes. Researchers have gained a better understanding of drug-target interactions and improved ability to design selective compounds. The improved prediction of potential side effects has led to safer drug development processes

4. Lead Optimization and Virtual Screening

4.1.1. Advanced Lead Optimization

Lead optimization represents a critical phase in drug development where promising drug candidates undergo molecular modifications to enhance their efficacy, stability, and selectivity [35]. Quantum computing accelerates this process through advanced molecular behavior simulations. The implementation of quantum algorithms like Quantum Monte Carlo (QMC) and quantum annealing has demonstrated superior effectiveness in optimizing molecular structures [36]. The integration of quantum computing in lead optimization has revolutionized traditional approaches by enabling more sophisticated analysis of structure-activity relationships. These advanced computational methods allow researchers to explore chemical spaces more thoroughly and predict molecular properties with unprecedented accuracy. The quantum-enhanced optimization process considers multiple parameters simultaneously, including binding affinity, metabolic stability, solubility, and potential toxicity.

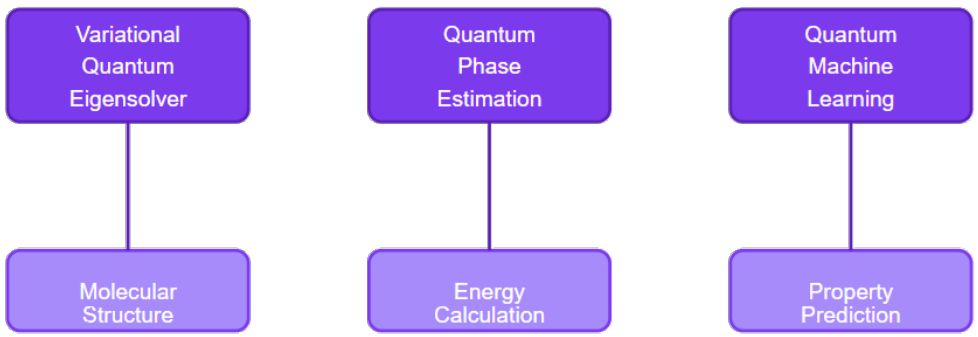

Figure 2. Quantum Algorithms

Several pharmaceutical companies have initiated quantum computing collaborations to leverage these capabilities. Notable partnerships include Pfizer's collaboration with IBM Watson Health for immuno-oncology research [37], and Boehringer Ingelheim's alliance with Google for molecular simulation applications [38]. D-Wave's quantum annealing technology has also shown significant progress in accelerating drug design optimization procedures [39].

Table 3. Major Quantum Computing Platforms and Their Applications in Drug Discovery

Platform Type	Companies	Drug Discovery Applications	Current Limitations
Superconducting Qubits	IBM, Google	Molecular simulation	Decoherence issues
Ion Trap	IonQ, Honeywell	Property calculation	Scaling challenges
Photonic	PsiQuantum, Xanadu	Quantum chemistry	Limited qubit connectivity
Quantum Annealing	D-Wave	Optimization problems	Limited problem types
Neutral Atoms	ColdQuanta	Atomic simulations	Early development stage

4.1.2. Virtual Screening Advancements

Quantum computing has transformed virtual screening processes by enabling efficient analysis of vast chemical compound databases. Traditional screening methods often struggle with the computational demands of evaluating millions of compounds [40]. Quantum-enhanced techniques, particularly Grover's search algorithm, have demonstrated superior efficiency in screening large compound libraries [41]. The implementation of quantum algorithms in virtual screening has significantly reduced the time and computational resources required for compound evaluation. This enhancement enables researchers to screen larger libraries of compounds more thoroughly, increasing the likelihood of identifying promising drug candidates. The quantum approach also improves the accuracy of screening results by incorporating more complex molecular interaction parameters and quantum mechanical effects.

4.2. Drug Repurposing and Bioactivity Prediction

4.2.1. Quantum-Enhanced Drug Repurposing

Drug repurposing, the identification of new therapeutic applications for existing drugs, has gained prominence as a cost-effective drug development strategy [42]. Quantum computers facilitate this process by modeling interactions between existing drugs and various biological targets [43]. This approach has proven particularly valuable in rapidly identifying potential treatments during health emergencies [44].

4.2.2. Advanced Binding Site Analysis

The quantum computing approach enables detailed analysis of binding site characteristics and drug-target interactions. This capability allows researchers to identify previously unknown binding possibilities and predict novel therapeutic applications for existing drugs. The enhanced computational power facilitates the evaluation of complex protein-ligand interactions across multiple therapeutic targets simultaneously.

4.2.3. Metabolic Pathway Modeling

Quantum computing enables comprehensive modeling of metabolic pathways and drug interactions within biological systems. This capability helps researchers understand how existing drugs might affect different pathways, leading to the discovery of new therapeutic applications. The technology allows for more accurate predictions of drug effects on various biological processes.

4.2.4. Prediction of Side Effect

The advanced computational capabilities of quantum systems enable better prediction of potential side effects and drug interactions. This feature is crucial in drug repurposing as it helps identify both beneficial and adverse effects of existing drugs in new therapeutic contexts. The technology allows for more comprehensive evaluation of drug safety profiles.

4.2.5. Population Response Analysis

Quantum computing facilitates the analysis of drug responses across diverse patient populations. This capability helps researchers identify specific patient groups that might benefit from repurposed drugs. The technology enables more precise predictions of drug efficacy in different demographic groups.

4.2.6. Resistance Mechanism Prediction

The quantum approach allows for better understanding and prediction of drug resistance mechanisms. This capability is crucial in identifying drugs that might remain effective against resistant disease variants. The technology enables researchers to anticipate and address potential resistance issues proactively.

4.2.7. Combination Therapy Optimization

Quantum computing supports the optimization of drug combinations in repurposing strategies. This capability helps researchers identify synergistic drug combinations that might enhance therapeutic outcomes. The technology enables more efficient evaluation of complex drug interaction patterns.

4.2.8. Economic Impact

The technology facilitates comprehensive analysis of the economic implications of drug repurposing. This includes evaluation of development costs, market potential, and comparative advantages over new drug development. The quantum approach enables more accurate prediction of commercial viability for repurposed drugs.

4.2.9. Regulatory Compliance

Quantum computing assists in analyzing regulatory requirements and compliance pathways for repurposed drugs. This capability helps streamline the approval process for new therapeutic applications of existing drugs. The technology enables more efficient navigation of regulatory frameworks in drug repurposing.

4.2.10. Clinical Trial Design

The quantum approach supports optimal design of clinical trials for repurposed drugs. This includes patient selection, dosing strategies, and endpoint determination. The technology enables more efficient and effective clinical evaluation of repurposed drug candidates

5. Integration of Computational Technologies

5.1. Hybrid Quantum-Classical Computing

The integration of quantum and classical computing creates a synergistic approach that maximizes the strengths of both technologies [45]. This hybrid model combines classical computing's capacity for handling large datasets with quantum computing's molecular simulation capabilities [46]. The integration represents a significant advancement in computational drug discovery, offering a practical solution to current technological limitations while leveraging the unique advantages of each computing paradigm.

This hybrid approach enables researchers to optimize resource allocation, utilizing classical computers for data preprocessing and management while employing quantum systems for complex molecular calculations. The synergy between these technologies has led to more efficient drug discovery processes, reducing computational overhead while maintaining high accuracy in molecular simulations.

5.1.1. Variational Quantum-Classical Algorithms

The Variational Quantum Eigensolver exemplifies successful hybrid implementation, combining quantum algorithms with classical optimization techniques [47]. This approach enables accurate electronic structure simulation while maintaining computational efficiency [48]. The integration of classical optimization methods with quantum computation has created a powerful framework for solving complex molecular problems.

These algorithms demonstrate remarkable versatility in handling various computational chemistry challenges. The classical component manages parameter optimization and data processing, while the quantum component tackles computationally intensive molecular calculations. This division of labor has proven particularly effective in reducing the quantum resources required while maintaining high accuracy in molecular simulations.

5.2. Machine Learning

5.2.1. Quantum Machine Learning

The convergence of quantum computing and machine learning has led to the emergence of Quantum Machine Learning (QML) [49]. QML algorithms enhance the predictive capabilities of quantum computers in various aspects of drug development. The technology has revolutionized bioactivity prediction for novel compounds, enabling more accurate assessment of potential drug candidates. Pattern recognition capabilities in molecular interactions have been significantly enhanced, leading to better understanding of drug-target relationships. The optimization of drug candidate structures has become more sophisticated through QML approaches, allowing for more efficient exploration of chemical spaces. The classification of potential therapeutic compounds has improved dramatically, enabling faster identification of promising drug candidates. These advancements have accelerated the drug discovery process while improving the accuracy of predictions.

Moreover, QML has enabled more sophisticated analysis of complex biological systems, leading to better understanding of disease mechanisms and potential therapeutic interventions. The technology has demonstrated particular strength in identifying subtle

patterns in molecular data that might be missed by conventional approaches. This enhanced pattern recognition capability has proven valuable in drug repurposing efforts and the identification of novel drug targets.

5.2.2. Predictive Modeling

The integration of machine learning with quantum computational workflows has significantly improved molecular simulation accuracy [50]. These integrated systems demonstrate superior performance in predicting drug-target interactions and identifying promising drug candidates [51]. The enhanced predictive modeling capabilities have transformed how researchers approach drug design and development.

The integrated technique enables more accurate prediction of drug properties, including absorption, distribution, metabolism, excretion, and toxicity (ADMET) characteristics. This improved predictive power has led to more efficient lead optimization processes and reduced failure rates in later stages of drug development. The technology has shown particular promise in predicting complex pharmacological properties that traditional computational methods struggle to assess accurately. Advanced predictive modeling techniques have also improved the understanding of structure-activity relationships, enabling more targeted drug design approaches. The integration of quantum computing with machine learning has enhanced the ability to predict drug resistance mechanisms and potential side effects, leading to more robust drug development strategies. The combination of these technologies has created a powerful platform for drug discovery, enabling more comprehensive analysis of molecular interactions and better prediction of therapeutic outcomes.

6. Challenges and Limitations

6.1. Technical Constraints

Current quantum computing systems face significant hardware limitations that affect their reliability and computational accuracy [52]. The primary challenge lies in the inherent sensitivity of quantum bits (qubits) to environmental interference. These qubits can lose their quantum states due to minimal external disturbances, leading to computational errors and reduced accuracy in molecular simulations [53]. The phenomenon of decoherence presents a particular obstacle in maintaining stable quantum states necessary for complex calculations [54].

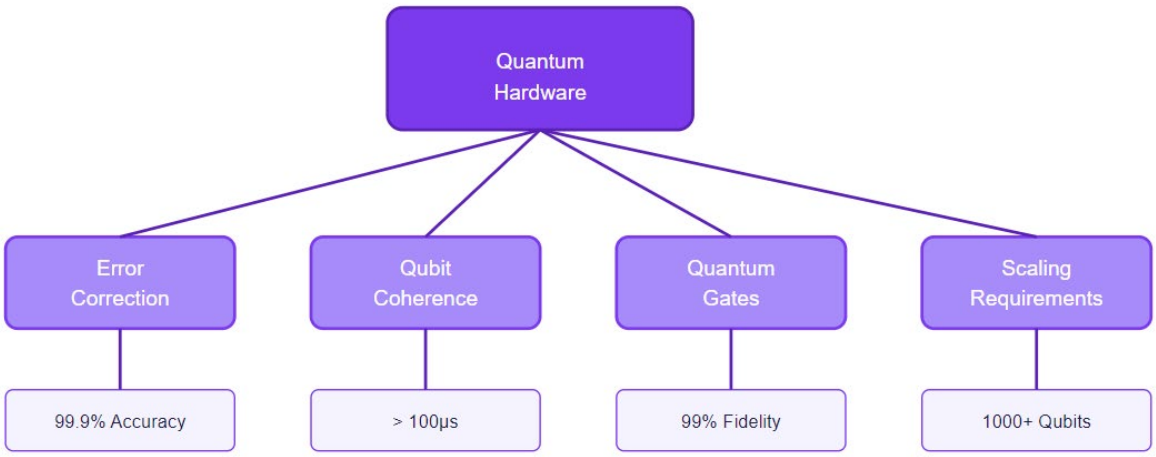

Figure 3. Quantum Hardware

The technical constraints extend beyond basic qubit stability issues. Temperature control requirements present significant operational challenges, as most quantum systems require extremely low temperatures to function effectively. This necessity for sophisticated cooling systems adds considerable complexity and cost to quantum computing infrastructure. Additionally, the scaling of quantum systems presents substantial engineering challenges, as increasing the number of qubits exponentially increases the complexity of maintaining quantum coherence.

Error correction mechanisms, while theoretically well-understood, remain practically challenging to implement at scale. The requirement for multiple physical qubits to create a single logical qubit significantly increases the hardware requirements for practical applications. Furthermore, the current generation of quantum computers struggles with noise accumulation during complex calculations, potentially limiting their utility in precise molecular modeling applications.

Table 4. Challenges and Solutions in Quantum Computing Implementation for Drug Discovery

Challenge Category	Specific Issues	Proposed Solutions
Technical	Qubit coherence	Error correction codes
	Quantum noise	Noise-resilient algorithms
Computational	Algorithm efficiency	Hybrid quantum-classical approaches
	Resource optimization	Better qubit utilization
Practical	Cost barriers	Cloud-based quantum services
	Expertise gap	Training programs

6.2. Algorithmic Development

The maturity of quantum algorithms remains a significant challenge in pharmaceutical applications. Current quantum algorithms designed for molecular simulations often lack the sophistication required for practical drug development applications [55]. The Variational Quantum Eigensolver, while promising, requires further optimization to effectively process the complex datasets typical in drug development workflows [56]. The development of more robust and efficient quantum algorithms represents an ongoing challenge in the field. The complexity of translating classical drug discovery algorithms into quantum-compatible versions presents significant theoretical and practical challenges. Researchers must balance the potential advantages of quantum computing with the limitations of current hardware capabilities. The optimization of quantum algorithms for specific pharmaceutical applications requires extensive experimentation and validation, often leading to lengthy development cycles.

Moreover, the integration of quantum algorithms with existing classical computational workflows presents additional challenges. The need to maintain consistency and accuracy while leveraging quantum advantages requires sophisticated hybrid approaches. The development of efficient error mitigation strategies for quantum algorithms remains an active area of research, particularly for applications requiring high precision.

6.3. Workforce Development

The pharmaceutical industry faces a substantial skills gap in quantum computing implementation [57]. The specialized nature of quantum computing requires expertise in quantum mechanics and computational chemistry, areas traditionally underrepresented in pharmaceutical education and training programs [58]. This knowledge gap creates significant obstacles for pharmaceutical companies attempting to integrate quantum computing into their existing research and development frameworks. The challenge extends beyond technical expertise to include the need for interdisciplinary knowledge spanning quantum physics, chemistry, biology, and computer science. The shortage of professionals with this diverse skill set hampers the effective implementation of quantum computing solutions in drug discovery. Additionally, the rapidly evolving nature of quantum technology requires continuous learning and adaptation, making it difficult for organizations to maintain up-to-date expertise.

Educational institutions face challenges in developing comprehensive quantum computing curricula that address the specific needs of the pharmaceutical industry. The lack of standardized training programs and certification frameworks further complicates workforce development efforts. Companies must invest significantly in internal training programs and partnerships with academic institutions to build and maintain necessary expertise.

6.4. Regulatory Guidelines

The regulatory guidelines for quantum computing applications in drug development remains largely unexplored compared to traditional drug discovery frameworks [59]. The main concerns include data privacy, algorithm transparency, and intellectual property rights. The absence of established regulatory guidelines for quantum-enhanced drug discovery presents challenges for pharmaceutical companies seeking to implement these technologies [60].

The complexity of quantum algorithms raises unique challenges for regulatory compliance and validation. Traditional validation methods may not be directly applicable to quantum computing processes, necessitating the development of new validation frameworks. The black-box nature of some quantum algorithms presents particular challenges for regulatory oversight and accountability. Data integrity and reproducibility requirements in pharmaceutical research create additional regulatory challenges for quantum computing applications. The probabilistic nature of quantum calculations may complicate efforts to meet stringent regulatory requirements for consistency and traceability. Furthermore, the international nature of drug development requires consideration of varying regulatory requirements across different jurisdictions.

The protection of intellectual property in quantum-enhanced drug discovery presents novel legal and regulatory challenges. The unique nature of quantum algorithms and their applications in drug discovery requires careful consideration of patent and trade

secret protection strategies. The global nature of pharmaceutical research necessitates consideration of international intellectual property laws and their application to quantum computing innovations.

7. Conclusion

The usage of quantum computing with existing computational methods has a significant potential in accelerating drug discovery processes and improving success rates. Applications ranging from structure-based drug design to drug repurposing showcase the versatility of quantum computing in pharmaceutical research. The synergy between quantum computing, classical computing, and machine learning has created powerful hybrid approaches that address complex challenges in drug development. These systems provide more accurate predictions of drug-target interactions and enable more efficient screening of potential drug candidates. Notable collaborations between pharmaceutical companies and quantum computing firms have already begun to yield practical applications in drug discovery workflows. While current limitations in hardware, algorithmic development, and workforce expertise present challenges, ongoing technologies and increasing industry adoption suggest a bright future.

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