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QUANTUM COMPUTING IN NEW DRUG DISCOVERY: A COMPREHENSIVE REVIEW

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ABSTRACT

The development of drugs has become more complicated over the past 40 years, necessitating the preclinical stage of drug research, an investigational new drug (IND) application, and lengthy clinical testing before receiving FDA marketing permission. Applications for new drugs (NDAs) or licenses for biologics (BLAs) are frequently carefully reviewed before approval. Drug performance is again presented to regulatory agencies for post-marketing research after authorisation. Quantum computing has emerged as a disruptive technology with the potential to revolutionize various fields, including drug discovery. The traditional process of discovering new drugs is a time-consuming and expensive endeavor, often requiring extensive computational resources to simulate and analyze molecular interactions. Quantum computing, with its ability to leverage quantum mechanics principles, offers new opportunities for accelerating drug discovery processes, enhancing molecular modeling, and improving the understanding of complex biological systems. This comprehensive review explores the application of quantum computing techniques and algorithms in the context of new drug discovery, highlighting key advancements, challenges, and future prospects.

Keywords: Quantum computing, Drug discovery, Computational chemistry, Quantum algorithms, Quantum machine learning, Quantum chemistry, Quantum molecular dynamics, Quantum optimization, Quantum-inspired algorithms, Quantum-enhanced drug discovery

1. INTRODUCTION

- **Overview of drug discovery process**

Over the past 40 years, the complexity of drug development has multiplied, necessitating the preclinical stage of drug research, an investigational new drug (IND) application, and extensive clinical testing prior to FDA marketing clearance. Before being approved, new drug applications

(NDAs) or biologics license applications (BLAs) are typically thoroughly scrutinized. Following approval, drug performance is then once again submitted to regulatory bodies for post-marketing research. The main objective is to provide patients with safer, more effective treatments as soon as possible following a careful medical review [1].

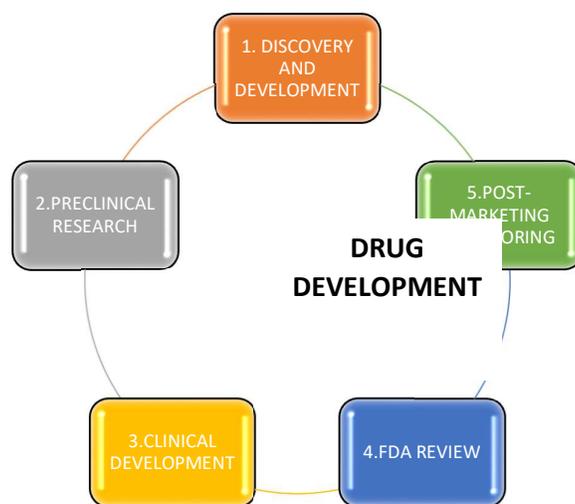


Figure 1: Process of Drug Development

Steps of Drug Discovery In Detail:

1. Discovery and Development:

First of all, target discovery is done. Target is a gene or a protein with some biological activity towards the disease researching about. After a target is being selected then target validation is done by the use of various tools and techniques like disease association, bioactive molecules, cell-based models, protein interactions, signalling pathways analysis, functional analysis of

genes, invitro genetic manipulation, antibodies, and chemical genomic [2].

After target validation, screening of compound is done to evaluate the drug's effect at cellular, molecular and biochemical levels. Through High Throughput Screening active compounds, genes or antibodies are identified. Then Hit to Lead process, is done on a small molecule selected from HTS and optimized to lead optimization process [1-2].

In lead optimization process, the lead compounds discovered are synthesized and modified to improve potency and reduce side-effects. In uses ADMET tools to

conduct experimental testing. Finally a API (Active Pharmaceutical Ingredient) is formed for next process of drug discovery and development [1].



Figure 2: Flowchart of Drug Discovery

2. Preclinical Research and FDA Review:

Before a medicine candidate is tested on humans, preclinical trials are designed to gather data on its safety and effectiveness. They typically consist of both in vitro and in vivo experiments and can also show the biological impact of the drug. Before submitting for approval as IND, preclinical research must follow the regulations set forth by Good Laboratory Practice in order to produce credible results⁵, which is why regulatory bodies like the FDA demand

them. Research on pharmacokinetics, pharmacodynamics, and toxicology offer information about the compound's dosage and toxicity levels, which is crucial for determining whether it is justified and relatively safe to move forward with clinical research [3].

3. Clinical Development:

After FDA approval, drug undergoes Clinical trials. Clinical Trial is conducted in following phases:

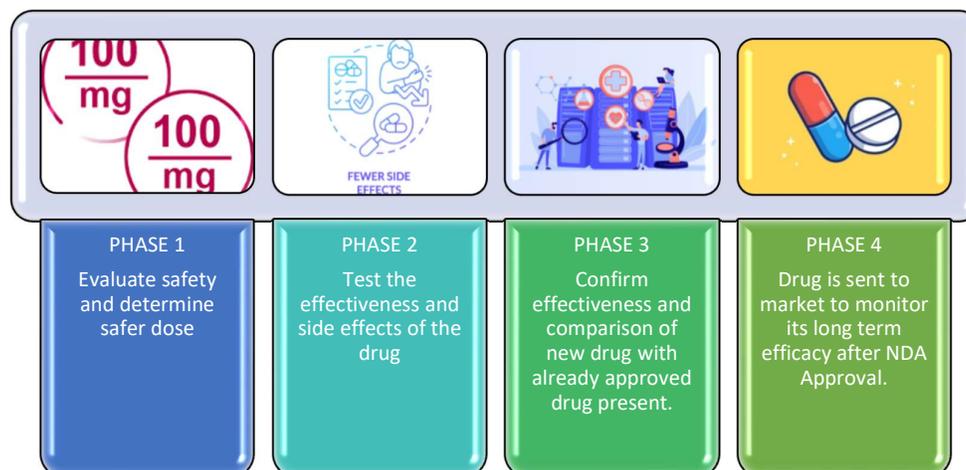


Figure 3: Phases of Clinical Trial

The above-mentioned process from discovery to approval, the expensive process

of drug discovery typically takes more than ten years. Notably, the cost and approval

time vary based on the ailment being treated and the medicine being developed. A treatment that is urgently needed and would typically go through a priority review process will have its review process take significantly longer than a drug that merely offers marginal enhancements over currently marketed therapies [4]. Additionally, producing an orphan drug (a medication for a rare or neglected medical condition) is substantially less expensive overall than developing a nonorphan medication [4]. For instance, the estimated cost of developing the medicine fexinidazole, which was licenced to treat the neglected condition known as sleeping sickness, was EUR 55 million [6], which is significantly lower than the nonorphan drug development cost that is estimated to exceed US\$2 billion [7].

However, modern advanced technologies are working to enable the creation of personalised therapies in addition to hastening the discovery process. Whole plant extracts are typically used in drug discovery, with single compound-based medicine as the driving force. Despite the fact that this resulted in the discovery of numerous effective therapies, these approaches frequently come with a number of difficulties that may lead to suboptimal biopharmaceutical or pharmaceutical performance, poor targeting, or formulation limitations [8]. These operations are no

longer used by current medical practises because they are unsustainable, regarded impracticable, and come with large related expenses. In order to accelerate the discovery process, industry research and development (R&D) is constantly evaluating new technologies and applications from various research disciplines. The pharmaceutical industry is still attempting to overcome the difficulty of finding a strong and viable lead medicine from the hit stage to drug candidate. As a result, drug development has undergone rapid changes that over the past few decades have led to substantial advancements in scientific research and technological innovation that have made it possible to quickly translate innovative drug ideas into usable entities. Drug development has been transformed by the capacity to create therapeutic molecules that are specifically targeted at a specific protein or biological function in a living cell. Additionally, the introduction of high throughput at various phases of drug discovery and development, as well as technological developments like the sequencing of the human genome, have significantly changed the way the process is carried out [8]. Such a step named Quantum Computing is now-a-days trending step for reducing the time and energy drug discovery and development process.

- **Quantum Computing and its principles**

In the field of pharmaceuticals, drug discovery is a complex and time-consuming process that involves the identification and development of new medications to treat various diseases and improve human health. This process typically takes several years and requires the collaboration of scientists, researchers, and clinicians from various disciplines.

Quantum computing, on the other hand, is an emerging field of study that harnesses the principles of quantum mechanics to perform computational tasks more efficiently than classical computers. Unlike classical computers that use bits to represent information as either a 0 or a 1, quantum

computers use quantum bits, or qubits, which can exist in superposition states of 0 and 1 simultaneously. This allows quantum computers to process and store a vast amount of information and perform complex calculations in parallel, potentially revolutionizing various industries, including drug discover [9].

In this discussion, we will explore the drug discovery process and provide an introduction to quantum computing and its underlying principles. We will highlight how quantum computing can potentially impact and accelerate drug discovery efforts, offering new possibilities for discovering novel medications and optimizing their development.

2. Quantum Computing Fundamentals

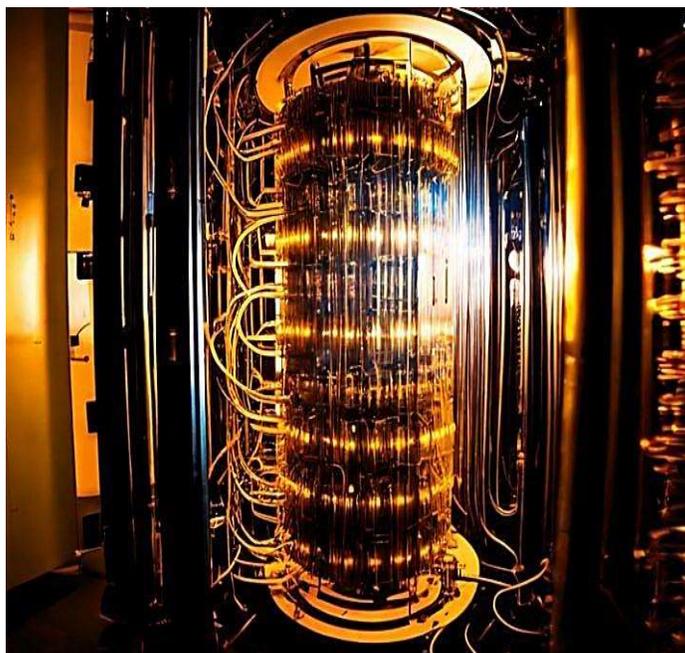


Figure 4: Quantum Computer

Brief overview of quantum mechanics principles

Quantum mechanics is a branch of physics that describes the behavior of particles at the atomic and subatomic level. It introduces a probabilistic understanding of nature, where particles can exist in multiple states simultaneously until observed or measured [10].

Quantum computing, focuses on the development of technologies based on the principles of quantum theory. Unlike classical computing technique, quantum computing uses the quantum physics technique to solve complex and time taking problems [11].

In the context of drug discovery, quantum mechanics is particularly relevant because it provides a more accurate description of molecular interactions and properties compared to classical physics. Quantum mechanics principles, such as the Schrödinger equation, enable the calculation of energy levels, molecular structures, and other properties that influence drug behavior and effectiveness [12].

- Quantum bits (qubits) and quantum gates

Unlike classical computers, Quantum computers does not use bits rather uses qubits. It is the fundamental unit of information, which can represent a superposition of both 0 and 1 simultaneously. This ability to exist in

multiple states simultaneously is crucial for performing parallel computations and exploring different possibilities simultaneously [13-14].

Unlike classical bits that can only represent a single value (either 0 or 1), qubits can represent both values simultaneously, thanks to the principle of superposition. Quantum gates are operations performed on qubits to manipulate and process quantum information. These gates can perform transformations that change the probabilities of measuring different states of the qubits [14].

- How Quantum Computer Works:

i. Superconductors

Like normal desktop computer requires fan to remain cool, quantum computers use super-cooled fluids to remain cool. Due to ultra-low temperature some materials exhibit important quantum mechanical effect hence called superconductors [15].

ii. Control

Josephson junctions are used as superconducting qubits. By firing photons at this qubits, a person can control the behaviour, and read individual units of quantum information [15].

iii. Quantum superposition

A qubit isn't particularly useful by itself. It can, however, pull off a crucial ruse by putting the quantum data it contains into a state of superposition that combines all qubit configurations that might be feasible.

Superposition of qubit groups can produce intricate, multidimensional computational landscapes. In these settings, complex issues can be represented in novel ways. Quantum superposition is a principle that allows qubits to be in a combination of multiple states simultaneously. For example, a qubit can exist in a superposition of being both 0 and 1 at the same time. This property is harnessed in quantum algorithms to perform computations on a massive scale by exploring many possible solutions simultaneously [15].

iv. Quantum entanglement

Quantum entanglement is a phenomenon where two or more qubits become correlated in such a way that the state of one qubit cannot be described independently of the state of the others. When qubits are entangled, measuring the state of one qubit instantaneously affects the state of the other, regardless of the distance between them. Entanglement allows for the creation of highly correlated quantum systems and is a crucial resource in quantum computing algorithms [16].

In drug discovery, quantum computing can leverage the principles of superposition and entanglement to perform complex simulations, optimize molecular structures, and solve computational challenges that arise in areas such as molecular dynamics simulations, drug target identification, and drug molecule optimization. By harnessing

the power of quantum mechanics, quantum computing has the potential to revolutionize the process of discovering new drugs and accelerating the development of personalized medicine.

v. Interference

There are waves of probability in a setting where entangled qubits are in a state of superposition. These are the likelihoods of the results of a system measurement. When several of these waves peak at the same result, they can build upon one another, or when peaks and troughs combine, they can cancel one another out. Both of these represent interference [15].

3. Quantum Computing Techniques in Drug Discovery

Quantum computing has the potential to revolutionize the field of drug discovery by offering faster and more accurate simulations, enabling advanced machine learning techniques, and providing novel optimization algorithms [17]. Here are some specific quantum computing techniques that are being explored in drug discovery:

- Molecular dynamics simulations using quantum computing

Quantum computers can be used to perform quantum molecular dynamics simulations, which model the behavior and interactions of atoms and molecules at the quantum level. These simulations can provide more accurate and detailed information about molecular structures, reactions, and

properties, leading to better understanding of drug-target interactions.

- Quantum machine learning for drug design and virtual screening

Quantum machine learning algorithms can leverage the unique properties of quantum systems to enhance drug design and virtual screening processes. Quantum computers can efficiently explore vast chemical spaces, enabling faster identification of potential drug candidates and predicting their properties and interactions with targets.

- Quantum algorithms for optimization and molecular property prediction

Quantum optimization algorithms, such as quantum annealing and variational quantum algorithms, can be applied to solve complex optimization problems encountered in drug discovery. These algorithms can help optimize drug candidates, design molecular structures with desired properties, and determine optimal conditions for synthesis or manufacturing processes.

- Quantum-inspired algorithms and their applications

Quantum-inspired algorithms, such as the Quantum Approximate Optimization Algorithm (QAOA), can be used on classical computers to tackle challenging optimization problems in drug discovery. These algorithms leverage principles inspired by quantum computing to improve the efficiency and accuracy of optimization

tasks, such as molecular property prediction and drug design.

It's worth noting that quantum computing is still in its early stages of development, and large-scale, fault-tolerant quantum computers are not yet widely available. However, researchers are actively exploring and developing these techniques to leverage the power of quantum computing in drug discovery. As the technology progresses, we can expect significant advancements in the field, leading to faster and more effective drug discovery and development processes [18].

4. Case Studies: Quantum Computing in Drug Discovery

QC has the potential to revolutionize drug discovery by enabling more efficient and accurate simulations of molecular interactions. While the field is still in its early stages, there have been several notable case studies exploring the applications of quantum computing in drug discovery. Here are two examples:

a. Simulation of Chemical Reactions:

In 2020, researchers from Google partnered with pharmaceutical company Amgen to study chemical reactions using a quantum computer. They focused on the Haber-Bosch process, which is used to produce ammonia, a key ingredient in fertilizers. By simulating the reaction using a quantum computer,

the researchers gained insights into the reaction mechanism at a molecular level. This understanding could potentially lead to the development of more efficient catalysts for ammonia production, which could have significant environmental and economic benefits [19].

b. Protein Folding and Drug Design:

In 2021, researchers from IBM Quantum collaborated with the University of Tokyo and the University of Oxford to investigate protein folding using quantum computing. Protein folding is a critical process that determines the structure and function of proteins, and understanding it is crucial for drug design. Traditional computational methods struggle to accurately simulate protein folding due to the complexity of the problem. The researchers used a quantum computer to simulate the folding process of small proteins, providing insights into the folding pathways and stable conformations. This information could aid in designing drugs that target specific protein structures and functions, potentially leading to more effective treatments for various diseases [19].

These case studies demonstrate the potential of quantum computing in drug discovery. However, it's important to note that quantum computers are still in the early stages of development, and large-scale quantum simulations for drug discovery are not yet feasible. Nonetheless, as quantum technology continues to advance, it holds great promise for accelerating the discovery and development of new drugs [20].

c. Structure based drug designing:

The target protein's structure is a crucial component of the input. On the basis of the amino acid sequence, some advancements in quantum approaches for protein folding have been made in the last ten years [21].

d. Molecular docking:

Atomistic modeling, which depends on force-field simplifications whose parameters must coincide with quantum-mechanical computations, is one of the most used techniques for molecular docking. The size of physical systems that can be treated with precise ab initio quantum calculations will be considerably increased as quantum devices scale up with the introduction of VQEs and the quantum phase estimation technique [21].

e. In denovo design:

One of the key concerns in de novo design is a drug candidate's capacity to be synthesized, which requires simulation of several chemical pathways. atomic computers provide a way to maybe address electronic structure utilizing issues in the strongly linked regime, which would permit us to replicate transitional phases and thermodynamic characteristics to FCI-like precisions methods. Consequently, this could increase the efficiency of new creation [21].

f. For ligand-based drug discovery:

In several instances, QSAR models have included quantum-mechanical features for ligand-based drug development. The effectiveness and predictability of the model are typically greatly influenced by the caliber and accuracy of these properties. The majority of these methods rely on descriptors produced from DFT calculations; quantum computation may provide a more accurate and efficient replacement for those calculations [21].

5. Challenges and Limitations

Quantum computing holds great promise for revolutionizing various fields, including drug discovery. However, there are several

challenges and limitations that need to be addressed before quantum computing can be fully integrated into the process of new drug discovery. Here are some of the key challenges:

- Hardware limitations and scalability issues

Quantum computers are still in the early stages of development, and the hardware available today has limited qubit counts and coherence times. To tackle the complexity of drug discovery, large-scale quantum computers with thousands or millions of qubits are required. Achieving this level of scalability is a significant challenge [16].

- Noise and error correction challenges

Quantum computers are highly susceptible to errors and noise due to interactions with the environment. Quantum error correction techniques are essential for reliable computations, but implementing error correction is a complex task. It requires additional qubits and sophisticated algorithms, which further exacerbate the scalability issues [16].

- Integration of quantum and classical computing systems

Drug discovery workflows typically involve a combination of classical and quantum computing tasks. Integrating quantum algorithms with classical computing systems poses challenges in terms of data transfer, communication, and synchronization between the two computing

paradigms. Efficient hybrid algorithms and software architectures need to be developed to address this integration challenge [16].

- Limited Quantum Algorithms for Drug Discovery

While quantum algorithms like the quantum variational eigensolver (QVE) and quantum phase estimation (QPE) have shown promise in simulating molecular systems, there is still a need for more robust and efficient quantum algorithms tailored specifically for drug discovery tasks. Developing these algorithms requires a deep understanding of the problem domain and exploiting the strengths of quantum computing [11].

- Data Access and Privacy Concerns

Drug discovery involves handling vast amounts of sensitive biological and chemical data. Sharing such data with external quantum computing providers may raise concerns about data privacy and security. Developing secure methods for data access and protection while leveraging the power of quantum computing is crucial [11].

- Cost and Accessibility

Quantum computers are currently expensive and challenging to access for most researchers and organizations. As quantum computing technology advances, efforts are being made to reduce costs and increase accessibility. However, making quantum computing more affordable and widely

available remains a significant challenge [11-16].

Addressing these challenges requires collaborations between researchers, industry experts, and policymakers. Continued research and development in quantum hardware, error correction techniques, hybrid computing architectures, and tailored algorithms are necessary to overcome the limitations and unlock the potential of quantum computing in new drug discovery.

6. Future Perspectives and Outlook

Quantum computing holds immense potential to revolutionize various fields, including drug discovery. Here are some perspectives on the potential impact of quantum computing on the drug discovery process, expected advancements in quantum hardware and algorithms, and the integration of quantum computing with other computational techniques.

- Potential impact of quantum computing on the drug discovery process [22]

Quantum computing can significantly accelerate the drug discovery process by tackling complex computational problems that classical computers struggle with. Some potential impacts include:

- a. **Molecular modeling and simulation:**
Quantum computers can simulate the behavior and properties of molecules more accurately, enabling researchers to understand drug interactions and design new molecules with specific properties.

This can expedite the discovery and optimization of drug candidates.

- b. Drug-target identification: Quantum algorithms can efficiently analyze vast biological datasets, such as genomics and proteomics, to identify potential drug targets. This can aid in identifying novel therapeutic targets and developing personalized medicines.
- c. Optimization of drug design: Quantum computers can perform complex optimization tasks, such as molecular structure optimization, to design drugs with improved efficacy and fewer side effects.
- d. Quantum machine learning: Quantum algorithms can enhance machine learning techniques, enabling more accurate prediction of drug properties and more efficient screening of large chemical libraries.

- Expected advancements in quantum hardware and algorithms [20-21]

Quantum computing is a rapidly evolving field, and several advancements can be expected in the near future:

- a. Increased qubit count: Quantum hardware is expected to scale up, leading to the creation of larger and more powerful quantum computers. This will enable the simulation of more complex molecular systems and accelerate the drug discovery process.

- b. Enhanced qubit coherence and error correction: Improvements in qubit coherence times and the development of robust error correction techniques will make quantum computations more reliable and accurate.
- c. Hybrid quantum-classical algorithms: The development of hybrid algorithms that combine classical and quantum computing techniques will enable the efficient utilization of quantum computers to solve complex drug discovery problems.
- d. Specialized quantum hardware: Hardware architectures specifically designed for pharmaceutical and drug discovery applications may emerge, tailored to exploit the unique advantages of quantum computing in this field.

- Integration of quantum computing with other computational techniques [21]

Quantum computing is not expected to replace classical computing entirely but rather complement it. Integration with other computational techniques can lead to synergistic effects:

- a. Hybrid quantum-classical workflows: Quantum computers can be used in combination with classical computers to solve specific drug discovery tasks efficiently. For example, quantum computers can generate molecular simulations or optimize drug candidates, while classical computers handle pre-

processing, post-processing, and result analysis.

- b. Quantum-inspired algorithms: Insights from quantum algorithms can inspire the development of classical algorithms with improved performance for drug discovery tasks. Classical algorithms can mimic some quantum features to enhance their capabilities.
- c. Quantum-enhanced machine learning: Quantum machine learning techniques can be integrated with classical machine learning methods to improve predictions of drug-target interactions, biomarker identification, and patient stratification.
- d. Data fusion and integration: Quantum computing can be combined with classical techniques for data integration from multiple sources, such as genomics, proteomics, and clinical data, enabling a more comprehensive understanding of disease mechanisms and personalized medicine.

- Promising future directions for quantum computing in drug discovery [20-21]

- a. Development of more powerful and reliable quantum hardware: Advancements in quantum technology are essential to overcome the current limitations in qubit coherence, gate errors, and scalability. Continued research and development efforts are needed to build more robust quantum

computers suitable for complex drug discovery applications.

- b. Expansion of quantum algorithms and software tools: Further exploration and refinement of quantum algorithms tailored specifically for drug discovery tasks are crucial. Additionally, the development of user-friendly software tools and platforms that integrate quantum computing with existing drug discovery workflows will democratize access to quantum resources.
- c. Collaboration between quantum scientists and drug discovery experts: Collaboration between quantum computing researchers and experts in drug discovery is essential to bridge the gap between theoretical advancements and practical applications. By combining domain expertise and quantum knowledge, innovative approaches can be developed to tackle specific drug discovery challenges.
- d. Integration of quantum computing with other emerging technologies: The integration of quantum computing with other emerging technologies, such as artificial intelligence (AI) and high-throughput experimentation, can amplify the capabilities of drug discovery processes. Synergistic applications of these technologies can lead to more efficient and accurate drug discovery pipelines.

Overall, the potential impact of quantum computing on the drug discovery process is substantial. As quantum hardware and algorithms continue to advance, and as integration with classical techniques progresses, we can expect significant breakthroughs in accelerating the discovery and development of new drugs and personalized therapies.

7. CONCLUSION

By providing a comprehensive overview of the application of quantum computing in new drug discovery, this review aims to shed light on the potential benefits, challenges, and future prospects of this emerging field. Researchers, scientists, and professionals in the pharmaceutical and computational chemistry domains will find this review valuable in understanding the current state and future implications of quantum computing in drug discovery.

QC has demonstrated great potential in addressing complex computational problems that are integral to drug discovery. Its ability to perform parallel computations and leverage quantum phenomena such as superposition and entanglement has the potential to accelerate the drug discovery process significantly. It can enhance molecular simulations and enable more accurate predictions of drug interactions with target molecules. By leveraging quantum algorithms, researchers can simulate molecular systems with greater

precision, leading to improved understanding of drug-target interactions, binding affinities, and drug efficacy.

Furthermore, quantum computing can facilitate the optimization of drug candidates. The ability to solve complex optimization problems more efficiently can accelerate the identification of lead compounds with desirable properties, such as high potency and low toxicity. Additionally, quantum machine learning algorithms can be applied to analyze large-scale molecular datasets and extract meaningful patterns. This can aid in the discovery of novel drug targets, prediction of drug toxicity, and optimization of drug dosing regimens.

Lastly, we can conclude that quantum computing holds significant promise in revolutionizing drug discovery. While there are still challenges to overcome, the advancements in hardware, algorithms, and interdisciplinary collaborations will drive the future development and application of quantum computing in this field. The potential to accelerate drug discovery timelines, optimize drug candidates, and enhance our understanding of complex molecular systems makes quantum computing an exciting frontier in pharmaceutical research.

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