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Quantum computing and AI in drug discovery and public health: Accelerating breakthroughs for global healthcare challenge

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Abstract

This paper explores the transformative power of revolutionizing healthcare through quantum computing and artificial intelligence (AI). The focus is on how these advanced technologies help drive drug discovery and public health strategies based on the premise that traditional methodologies for developing drugs have become inefficient, especially with a very low success rate for viable therapy. Thus, there is a need for innovative techniques capable of enhancing the effectiveness of the process. Quantum computing enables simulations and complex calculations that are not achievable using traditional computers, providing more efficient ways to identify more effective therapies and drug candidates. The combination of AI-powered algorithms to optimize predictive analytics, this capability is poised to improve public health outcomes while shortening timelines for drug discovery. Using empirical evidence backed up by case studies, this study finds that these technologies can expedite new medication development while supporting healthcare systems to address the pressing concern of ageing populations and emerging diseases. Although some challenges exist with integrating these technologies, including technical limitations and ethical concerns like data privacy, experts are finding ways to balance the potential of quantum computing and AI to protect individual patients' rights and provide equitable access to real-time healthcare solutions.

Keywords: Quantum Computing; Artificial Intelligence; Drug Discovery; Public Health; Global Healthcare.

1. Introduction

Drug discovery and public health grapple with global healthcare challenges. Likewise, there is a mismatch between current efforts targeted at drug development, with a disproportionate focus on oncology and healthcare priorities in many parts of the world [1]. The drug discovery process is complex, collaboration-inclined, and resource-intensive across disciplines such as chemistry, toxicology, and biology [2]. In Asia, especially in China, challenges like the need for improved documentation of efficacy and adverse impacts in Chinese-based proprietary medicines, pharmacogenetic variances, and the concurrent use of Chinese and Western medicines remain [3]. Similarly, market-driven drug discovery is not feasible for tropical diseases affecting millions of people in low-income economies, hence the need for public-private partnerships.

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Emerging technologies, however, are critical for addressing these numerous healthcare challenges of public health and drug discovery. AI, the Internet of Things (IoT), blockchain, nanotechnology, and wearable devices offer opportunities to enhance population health, tackle pandemic challenges, and enhance cancer prevention [2]. Likewise, blockchain and AI can revolutionize the methods and processes of epidemiology in disease surveillance, enabling customized health communication, real-time monitoring of environmental conditions, and improved infectious disease management [4].

Quantum computing and artificial intelligence (AI) will revolutionize healthcare and drug discovery, providing tremendous capabilities in data analysis, molecular simulation, and optimization [5]. Through these technologies, [6] wrote that experts and industries can accelerate the drug development process by reducing costs & time and improving success rates. Quantum algorithms such as quantum machine learning models and variational quantum eigensolvers (VQE) are applied to resolve issues regarding the simulation of biological systems and sensitive data management [5].

This paper aims to explore how quantum computing and artificial intelligence (AI) are revolutionizing drug discovery and public health through accelerated research, improved predictive modelling, and overcoming traditional computational limitations.

The objectives are to:

- To explore the limitations of traditional drug discovery and public health strategies and how quantum computing and AI can address these challenges
- To assess the role of quantum computing and AI in accelerating drug discovery and improving public health outcomes
- To evaluate real-world applications and case studies highlighting how leading organizations adopt the technologies for pharmaceutical innovation
- To identify key challenges, ethical considerations and policy recommendations for effective integration of quantum computing and AI in healthcare.

2. Quantum Computing and AI in Drug Discovery and Public Health

2.1. Current Challenges in Drug Discovery and Public Health

Significant challenges remain in drug discovery and development, for example, high costs of $800 million - $1.9 billion, complexity, and lengthy timelines [7] Traditional drug development methods are inadequate to address and understand disease mechanisms and effective treatments for different conditions [8]. To overcome these obstacles, collaborative techniques involving academic institutions, pharmaceutical companies, clinicians, funding agencies, and multi-national consortiums must share knowledge, risks, and resources. In addition, AI and machine learning (ML) technologies are being proposed to improve efficiency, accelerate drug discovery processes, and solve various health problems [9]. These advanced computational methods have the potential to handle volumes of biological data and develop algorithms for drug testing & design to reduce costs and time associated with traditional drug development techniques.

Furthermore, in line with limitations in outbreak prediction and disease modelling, while predictive modelling for disease infestation depends on different data sources and advanced techniques, they face the challenge of model complexity and data quality [10]. Data scarcity usually prevents effective mathematical models for new pathogens, although the increasing availability of ecological and genetic data is enabling their potential [11]. Therefore, shifting to broader system vulnerability identification, which transcends mere prediction of individual disease patterns, is proposed to provide cross-cutting solutions. Cost, time, and risk obstacles facing drug development necessitate novel technologies and efficient strategies [8].

2.2. Quantum Computing in Drug Discovery

Quantum computing has great potential to transform drug discovery through principles of entanglement and superposition. With such technology, experts in the field can carry out complex calculations more rapidly and effectively than is obtainable with classical computers. [12] opined that this would enable efficient chemical compound screening and drug candidates' optimization. Quantum computers can leverage qubits existing in different states for substantive parallel processing [13].

Some common applications in drug discovery are molecular docking, protein folding, and artificial intelligence-based optimization [14]. Quantum computing offers loads of benefits, providing solutions for delicate biological problems. However, [12] observed that developing specialized software and algorithms remains a challenge, which may be resolved in future by integrating classical and quantum computing, AI, and ML solutions for drug discovery activities [15]. Furthermore, quantum computing can enable molecular simulations and accurate prediction of drug-target interactions [2]. Quantum simulation and machine learning, especially hybrid quantum-classical methods show potential with intermediate-scale devices [16].

2.3. AI in Drug Discovery and Public Health

Artificial intelligence (AI) is revolutionizing personalized medicine and drug discovery. Technologies like deep learning and machine learning are being adopted by the drug and healthcare industries to accelerate the development of new therapeutics [4]. Through these approaches, large-scale omics data and e-health records can be analyzed, while enabling precision medicine strategies and biomarker discovery [17]. AI-driven methods are beneficial for clinical trial design and target identification for advanced treatment approaches. Meanwhile, according to [18], integrating AI in drug discovery is predicted to revolutionize modern medicine by taking advantage of the full molecular profile of the patient - which transcends conventional biomarker-based techniques. In addition, AI algorithms are deployed for designing new drug candidates, predicting their metabolism & safety, and engineering delivery systems [19]. Integrating AI in drug discovery and to the broader public health promises to demonstrate a significant impact on clinical practice while accelerating personalized therapies.

2.4. Synergies Between AI and Quantum Computing

Quantum machine learning (QML) is effective for exploring the quantum computing-AI interaction, enhancing learning agents while providing speed-ups for data analysis [16] [20]. Quantum computing can shorten drug discovery timelines and quantum-enhanced technique fosters precise drug interactions prediction and molecular-level designs [21]. In addition, integrating quantum sensors with artificial intelligence can facilitate the detection of subtle abnormalities and medical imaging. [2] argued that the advancement of quantum adware will compel hybrid quantum-classical techniques for machine learning and quantum simulation to ensure near-team applications through noisy intermediate-scale quantum devices.

3. Case Study Analysis

3.1. Case Study 1: Pfizer & IBM's Quantum Computing Collaboration

Integrating quantum computing and drug development could be viable for addressing challenges related to drug-target interaction prediction and clinical trial outcomes optimization. This will potentially accelerate the drug development process [22]. Pfizer's and IBM's collaboration on the use of quantum computing for molecular simulations in drug discovery is noteworthy.

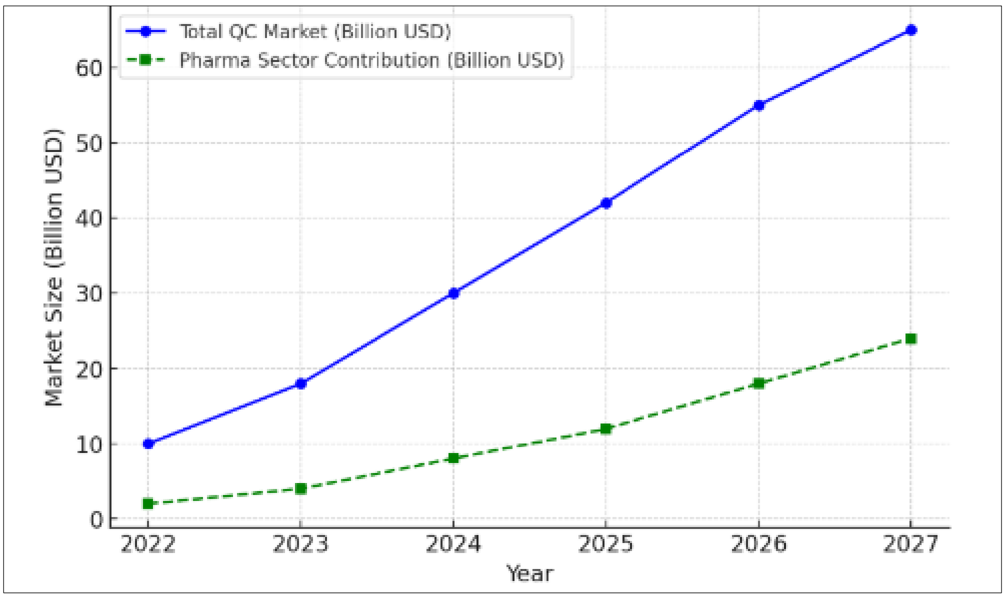

Figure 1 Global quantum computing market projection (2022-2027)

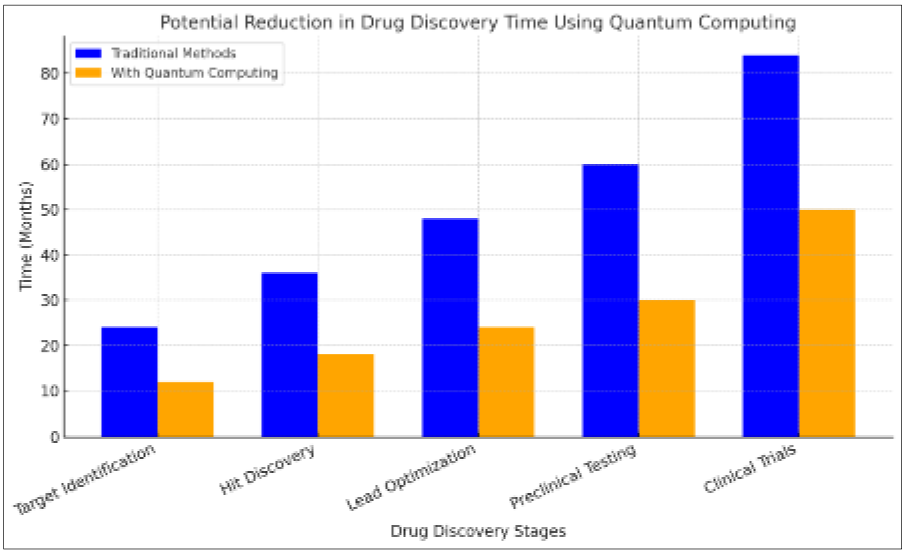

Figure 2 Potential reduction in drug discovery time using quantum computing [Evidence of Pfizer's & IBM's Quantum Computing collaboration]

While some challenges were observed with the practical implementation of this advanced technology including data quality and quantity, scalability, and quantum noise & error correction, the overall future outlook of the collaboration shows the transformative power of quantum computing with projected advancements in areas like rapid vaccine development, complex disease modelling, precision medicine, and personalized treatment methods [23].

3.2. Case Study 2: BenevolentAI and AI-Driven Drug Discovery

BenevolentAI, as a leading AI-powered drug discovery company, leverages machine learning (ML) to identify potential areas to apply therapy for existing drugs. The most notable success it has recorded over the years is the identification of *Baricitinib*, a Janus kinase (JAK) inhibitor which was originally developed for treating rheumatoid arthritis and potentially considered for COVID-19. The drug has been tested and gained Emergency Use Authorization (EUA) from the US FDA, with clinical trials showing the role of *baricitinib* in reducing mortality rates by 38% among COVID-19 patients when used with other standard treatments. Generally, although this provides another evidence of the role of AI in improving drug discovery, quantum computing could also improve AI-powered drug redirecting and repurposing by improving target identification, accelerating molecular simulations, and reducing drug repurposing timelines.

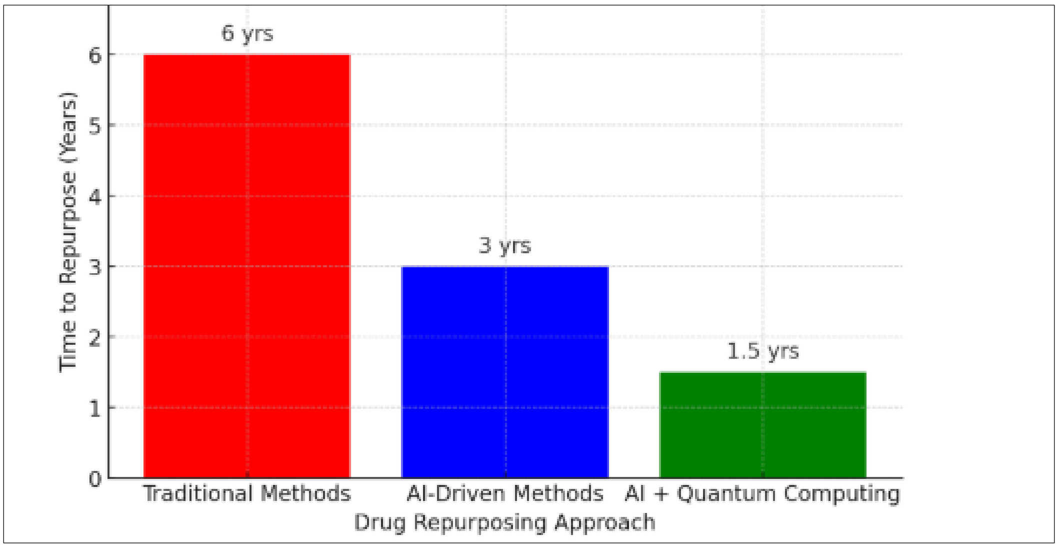

Figure 3 Reduced drug repurposing time with AI & Quantum Computing

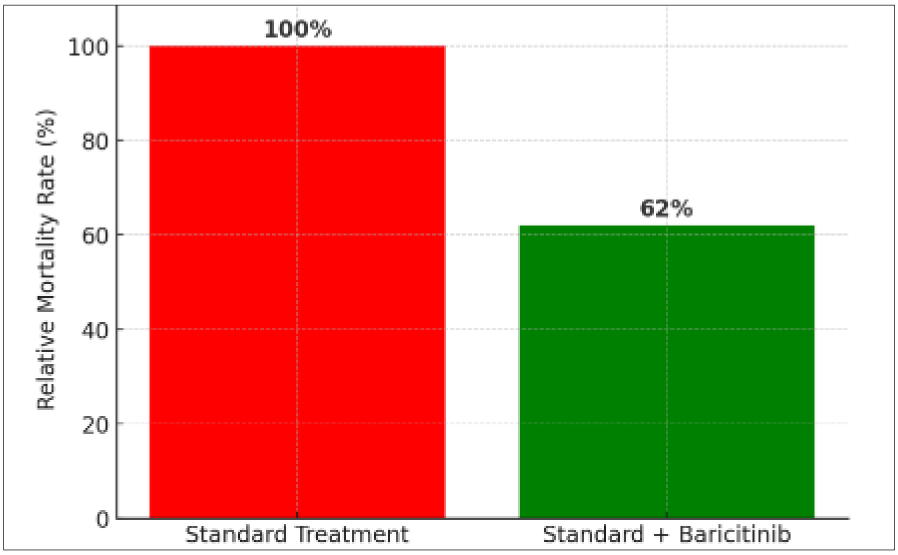

Figure 4 Impact of *Baricitinib* on COVID-19 mortality reduction

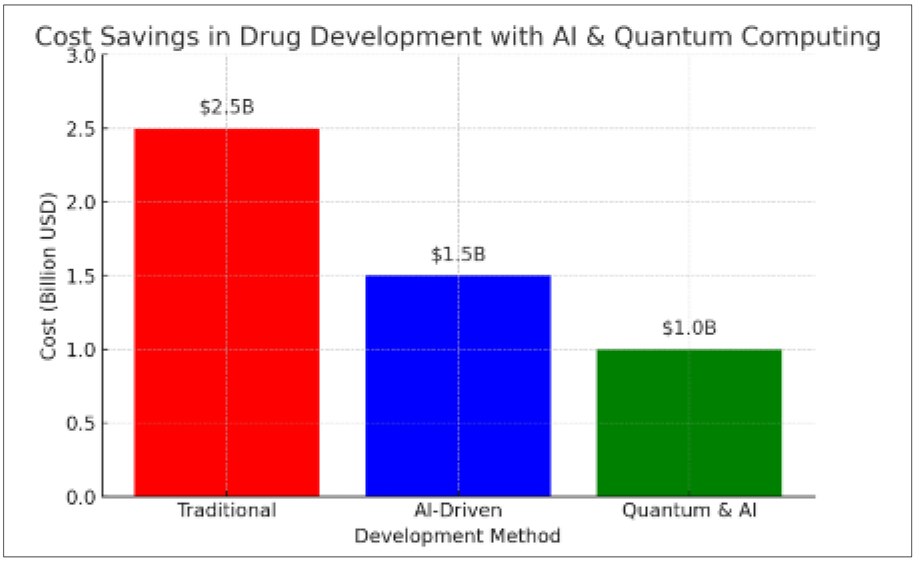

Figure 5 Cost savings in drug development with artificial intelligence and quantum computing

4. Challenges and Limitations

Quantum computing holds great potential and promises to accelerate drug discovery and development while addressing related challenges and enhancing efficiency to reduce costs and time to bring new drugs to market [15]. Challenges like computational complexity and hardware constraints, however, exist. First, the noisy intermediate-scale quantum (NISQ) era methods are limited to addressing drug discovery problems like molecular docking and protein folding. Although integrating quantum computing and classical computing, artificial intelligence, and machine learning may help to overcome these challenges, quantum machine learning algorithms like Deep Neural Networks and Support Vector Machines in drug discovery applications set the tone for future innovations in the field [24].

Furthermore, the effective application of quantum computing can be hampered by the need for high-quality data in areas with prevalent neglected diseases [25]. Therefore, ethical concerns like bias mitigation and data privacy need to be carefully considered [26-30]. Similarly, regulatory gaps have been identified as existing policies seem inadequate to keep pace with advancing AI applications, hence the need for effective guidelines and harmonized frameworks for higher transparency, safety, and equitable treatment [31-33]. To overcome these challenges, explainable AI, data augmentation, and integration with other traditional experimental methods can prove useful.

5. Conclusion and Recommendations

In conclusion, this research paper examines how quantum computing combined with artificial intelligence (AI) can revolutionize both drug discovery and public health systems. The conventional methods of drug development are considered sluggish, expensive, and ineffective, while quantum computing facilitates extraordinary molecular simulations alongside intricate computations. AI also boosts predictive modelling to speed up drug repurposing. The partnership between Pfizer and IBM, and Benevolent AI's achievements with Baricitinib showcase how these technologies shorten development periods while decreasing expenses and enhancing treatment effectiveness.

Quantum hardware constraints alongside data quality issues, ethical concerns, and regulatory deficiencies need resolution to achieve full potential benefits. Quantum computing and AI present a vast potential for future advancements such as swift vaccine creation, precision healthcare, and sophisticated disease modelling. Hybrid quantum-classical algorithms with explainable AI help deliver dependable and scalable healthcare applications. To secure data privacy, reduce bias, and foster equal access to these advancements, policymakers need to develop strong regulatory structures. Governments, academia and pharmaceutical companies must engage in international collaboration to harmonize standards and promote responsible adoption.

In essence, these technologies require interdisciplinary research from quantum physics, bioinformatics, and AI ethics to reach their full potential. The development of quantum infrastructure with high-quality datasets and workforce training will speed progress. Integrating quantum-AI technologies by overcoming present barriers and promoting international collaboration can initiate a revolutionary healthcare period, providing accelerated treatment development while ensuring safety and efficacy for worldwide health issues.

Compliance with ethical standards

Disclosure of conflict of interest

No conflict of interest to be disclosed.

Authors' Contribution

- **Teckla Tifuh Njei** contributed to the conceptual framework and literature review on quantum computing in drug discovery.
- **Taiwo Dolapo Oluyemo** served as the corresponding author and led the manuscript drafting and editorial coordination.
- **Oladipo Israel Owoyomi** provided the public health perspective and synthesized case studies on disease modelling and predictive analytics.
- ***Victoria Ronke Olatunde*** *contributed expert insights on neurological healthcare applications and reviewed the manuscript for clinical relevance*
- ***Odetoran Akinrotimi*** *analyzed AI and quantum synergies, contributing technical insights and model validation.*
- **Gbenga John Ilori** assisted in data gathering, proofreading, and formatting of figures and references.

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