Journal of Neonatal Surgery
ISSN(Online): 2226-0439
Vol. 14, Issue 21s (2025)
https://www.jneonatalsurg.com

OPEN ACCESS

Exploring the Potential of Quantum Computing for Drug Design

Surbhi Kamboj[1], Gorika Tomar[2], Archana[3], Km. Saiphali[4], Sohom Mukherjee[5], Arjun[6], Kunal[7*], Stuti Pandey[8]

[1]KIET School of Pharmacy, KIET Group of Institutions, Ghaziabad

[2]Dev Bhoomi Uttarakhand University, Dehradun, Uttarakhand, India

[3]Assistant Professor (Pharmacognosy), Panipat institute of engineering and technology Panipat, Haryana

[4]Panipat institute of engineering and technology, Panipat Haryana

[5]PhD Research scholar, MCOPS, Manipal Academy of Higher Education, Manipal, Udippi, India.

[6]Data Analyst - Data Engineering, Innovaccer, Sector 62, Noida, Uttar Pradesh 201309

[*7]R.P. Educational Trust Group of Institutions Bastara, Karnal

[8]Professor, Vandana Institute of Pharmacy, Ghazipur, Uttar Pradesh

Corresponding Author: Kunal

Email ID: Kunal7419028442@gmail.com

Cite this paper as: Surbhi Kamboj, Gorika Tomar, Archana, Km. Saiphali, Sohom Mukherjee, Arjun, Kunal, (2025). Exploring the Potential of Quantum Computing for Drug Design. *Journal of Neonatal Surgery*, 14 (21s), 1012-1024.

ABSTRACT

Quantum AI, the integration of quantum computing and artificial intelligence, is revolutionizing drug design by addressing the limitations of traditional pharmaceutical development. This review explores its transformative potential in enhancing molecular simulations, structure-based, target-based, and ligand-based drug discovery, and personalized medicine. Quantum computing leverages principles like superposition, entanglement, and interference to perform complex calculations exponentially faster than classical systems, enabling precise modeling of molecular interactions. Algorithms such as the Variational Quantum Eigensolver (VQE) and Quantum Phase Estimation (QPE) outperform classical methods like Density Functional Theory (DFT) in accuracy and efficiency, facilitating the identification of promising drug candidates and optimizing their pharmacokinetic properties. Quantum AI also enhances personalized medicine by analyzing vast genomic datasets to tailor treatments, improving efficacy and minimizing adverse effects. Despite challenges, including noisy intermediate-scale quantum (NISQ) device limitations and the need for advanced error correction, ongoing research and interdisciplinary collaboration are driving progress. Quantum AI promises to reduce development costs, accelerate drug discovery, and democratize access to life-saving medications. By enabling simulation-based discovery and expanding drug-candidate libraries to include peptides and antibodies, it paves the way for breakthroughs in treating complex diseases. This review underscores the need for continued investment in quantum technology to fully harness its potential, positioning the pharmaceutical industry for a future where drug development is faster, more precise, and patient-centric, ultimately improving global healthcare outcomes.

Keywords: *Quantum AI, Drug Discovery, Molecular Simulations, Personalized Medicine, Variational Quantum Eigensolver.*

INTRODUCTION:

Quantum AI, a synergy of quantum computing and artificial intelligence, is poised to transform the pharmaceutical industry by revolutionizing drug design and discovery[1]. This integration leverages the unparalleled computational power of quantum computing to solve complex molecular interactions that are challenging for classical computers, while AI enhances predictive capabilities and data analysis[2]. The background of this integration is rooted in the limitations of traditional drug development processes, which are often time-consuming and costly due to extensive experimentation and trial-and-error approaches[3]. Quantum AI addresses these limitations by enhancing the accuracy and speed of molecular modeling and simulation, crucial for understanding drug-target interactions and optimizing drug candidates[4,5]. The aim of this exploration is to delve into the potential of Quantum AI in drug design, examining how it can streamline the discovery process, improve the efficacy of drug candidates, and reduce development costs[3]. This is achieved through advanced quantum algorithms like the Variational Quantum Eigensolver (VQE), which can outperform classical methods such as Density Functional Theory (DFT) in terms of accuracy and efficiency in quantum chemical calculations[6]. The significance of Quantum AI in the pharmaceutical industry cannot be overstated, as it holds the potential to revolutionize drug discovery by enabling the simulation of complex molecular interactions that are beyond the capabilities of classical computers[7],[2]. This could lead to breakthroughs in treating diseases more effectively and efficiently, thereby improving patient outcomes and healthcare systems globally[8]. By leveraging Quantum AI, pharmaceutical companies can accelerate the identification of promising drug candidates, optimize their pharmacokinetic properties, and predict potential side effects more accurately[9]. Furthermore, Quantum AI can facilitate personalized medicine by analyzing vast amounts of patient data to tailor treatments to individual needs, enhancing treatment efficacy and patient adherence[10]. As Quantum AI continues to evolve, it is expected to play a pivotal role in shifting the pharmaceutical industry towards more simulation-based drug discovery processes, reducing reliance on empirical methods and enhancing the overall efficiency of drug development pipelines[11]. This shift will not only benefit pharmaceutical companies by reducing costs and improving success rates but also contribute to societal well-being by making life-saving medications more accessible and affordable [1,6].

The integration of Quantum AI into drug design also underscores the importance of interdisciplinary collaboration between quantum physicists, AI researchers, and pharmaceutical scientists to fully harness its potential[12]. Despite the challenges associated with implementing Quantum AI in legacy systems and addressing ethical considerations, the long-term benefits are substantial, positioning early adopters for significant competitive advantages in the future[13,9]. As the technology matures, it is crucial for stakeholders to invest in research and development, ensuring that Quantum AI is harnessed responsibly and effectively to transform the pharmaceutical landscape[14,5]. By embracing this cutting-edge technology, the pharmaceutical industry can embark on a new era of innovation, where drug discovery is faster, more precise, and more patient-centric than ever before[15]. Ultimately, the convergence of Quantum AI and pharmaceuticals represents a groundbreaking opportunity to redefine the drug development process, promising a future where treatments are more effective, safer, and tailored to individual patient needs, thereby revolutionizing healthcare outcomes worldwide[10,8]. Quantum AI also enables the creation of new types of drug-candidate libraries that are no longer restricted to small molecules but also include peptides and antibodies, allowing for a more automated approach to drug discovery[16]. Additionally, Quantum AI can enhance our understanding of drug-target interactions through QM/MM (Quantum Mechanics/Molecular Mechanics) simulations, which are vital in the post-drug-design computational validation phase[17]. This development not only facilitates a detailed examination of covalent inhibitors but also propels the field of computational drug development forward[18]. Through these advancements, Quantum AI is set to transform the drug discovery landscape by making it more efficient, accurate, and personalized, leading to better health outcomes and improved quality of life for patients globally[19]. As Quantum AI continues to evolve, its impact on the pharmaceutical industry will be profound, enabling faster and more accurate drug discovery processes that can address complex health challenges more effectively than ever before[20,14].

Fundamentals of Quantum Computing:

Quantum computing is a revolutionary technology that leverages the principles of quantum mechanics to perform calculations exponentially faster than classical computers[21]. At its core, quantum computing relies on three fundamental principles: superposition, entanglement, and interference[22]. Superposition allows qubits, the quantum equivalent of classical bits, to exist in multiple states simultaneously, enabling quantum computers to explore a vast solution space in parallel[23]. This property is crucial for solving complex problems that are intractable for classical systems[24,16]. Entanglement, another key principle, connects qubits in such a way that the state of one qubit is directly correlated with the state of another, even when separated by large distances[25]. This phenomenon facilitates highly efficient and coordinated computations[26,15]. Interference, the third principle, allows quantum states to interact and cancel out incorrect solutions while amplifying correct ones, enhancing the accuracy of quantum computations[27]. Quantum computing harnesses these principles to solve problems in fields like cryptography, optimization, and drug discovery, where classical computers struggle[28]. In the context of drug design, quantum computing can significantly enhance the efficiency and accuracy of molecular simulations and machine learning tasks[15]. Key quantum algorithms relevant to drug design include quantum machine learning and quantum simulations[11]. Quantum machine learning algorithms, such as Quantum Support Vector Machines (QSVM) and Quantum k-Means (Qk-Means), can process vast amounts of data more efficiently than their classical counterparts, enabling faster identification of promising drug candidates[20]. Quantum simulations, particularly those using the Variational Quantum Eigensolver (VQE), can accurately model complex molecular interactions, crucial for understanding drug-target binding and optimizing drug efficacy[4]. These simulations can also predict potential side effects more accurately, leading to safer drugs[18]. Additionally, quantum algorithms like the Quantum Approximate Optimization Algorithm (QAOA) can be used to optimize drug design by solving complex optimization problems that arise in the drug discovery process[12],[19]. The integration of quantum computing into drug design not only accelerates the discovery process but also enhances the precision of drug development, potentially leading to breakthroughs in treating complex diseases[16,29]. As quantum computing continues to evolve, it is poised to revolutionize the pharmaceutical industry by making drug discovery faster, more efficient, and more personalized[30]. This transformation will rely on the continued development of quantum algorithms tailored to pharmaceutical applications and advancements in quantum hardware to support these complex computations[31,20]. Furthermore, the collaboration between quantum physicists, AI researchers, and pharmaceutical scientists will be essential in fully harnessing the potential of quantum computing in drug design[32]. Despite the challenges associated with implementing quantum computing in legacy systems and addressing ethical considerations, the long-term benefits are substantial, positioning early adopters for significant competitive advantages in the future[22],[31]. As the technology matures, it is crucial for stakeholders to invest in research and development, ensuring that quantum computing is harnessed responsibly and effectively to transform the pharmaceutical landscape[27]. By embracing this cutting-edge technology, the pharmaceutical industry can embark on a new era of innovation, where drug discovery is faster, more precise, and more patient-centric than ever before[19,32]. Ultimately, the convergence of quantum computing and pharmaceuticals represents a groundbreaking opportunity to redefine the drug development process, promising a future where treatments are more effective, safer, and tailored to individual patient needs, thereby revolutionizing healthcare outcomes worldwide[33]. Quantum computing also enables the creation of new types of drug-candidate libraries that are no longer restricted to small molecules but also include peptides and antibodies, allowing for a more automated approach to drug discovery[34,13]. Additionally, quantum simulations can enhance our understanding of drug-target interactions through QM/MM (Quantum Mechanics/Molecular Mechanics) simulations, which are vital in the post-drug-design computational validation phase[35]. This development not only facilitates a detailed examination of covalent inhibitors but also propels the field of computational drug development forward[36],[16]. Through these advancements, quantum computing is set to transform the drug discovery landscape by making it more efficient, accurate, and personalized, leading to better health outcomes and improved quality of life for patients globally[37]. As quantum computing continues to evolve, its impact on the pharmaceutical industry will be profound, enabling faster and more accurate drug discovery processes that can address complex health challenges more effectively than ever before[23,29]. The integration of quantum computing into pharmaceutical research also underscores the importance of interdisciplinary collaboration and investment in quantum technology to fully realize its potential in drug design and development[38,39].

Applications of Quantum AI in Drug Discovery:

Quantum AI is applied in drug discovery to enhance molecular simulations and machine learning, enabling faster and more accurate identification of promising drug candidates by simulating complex molecular interactions[7]. Additionally, Quantum AI facilitates personalized medicine by analyzing vast patient data, optimizing drug efficacy, and predicting potential side effects more accurately, leading to safer and more effective treatments[40].

Molecular Simulations:

Quantum simulations have emerged as a transformative tool in modeling molecular interactions with unprecedented accuracy, revolutionizing the field of drug discovery[37]. Traditional computational methods, such as classical molecular dynamics and density functional theory (DFT), struggle to handle the complexity of quantum mechanical interactions within large biological molecules due to computational limitations and the need for empirical approximations. Quantum simulations, leveraging principles like superposition and entanglement, offer a fundamentally different approach by naturally incorporating quantum effects, enabling the efficient modeling of complex molecular behavior[19]. One of the key quantum algorithms used in molecular simulations is the Variational Quantum Eigensolver (VQE). VQE is a hybrid quantum-classical approach that finds the ground-state energy of molecular systems by iteratively optimizing parameters to minimize energy[39]. This method is particularly useful in drug discovery, where understanding the electronic structure of molecules is crucial for predicting binding affinities and reaction mechanisms[18]. For instance, researchers have successfully applied VQE to simulate complex molecular interactions in proteins like hemocyanin, which is involved in oxygen transport and cancer vaccine development[20]. Another powerful quantum algorithm is Quantum Phase Estimation (QPE), which directly computes eigenvalues of a Hamiltonian, providing exact results but requiring more qubits and longer coherence times[41,23]. Once error-corrected quantum computers become viable, QPE could offer highly accurate simulations of molecular interactions, further enhancing drug discovery capabilities[17]. Additionally, Quantum Monte Carlo (QMC) methods can be adapted to quantum computers to improve sampling of molecular configurations, enhancing protein folding predictions and ligand-protein interactions[42]. Quantum simulations have already demonstrated significant progress in modeling complex molecular systems. For example, researchers have used quantum-centric simulations to study noncovalent interactions between molecules, achieving remarkable agreement with classical methods like CASCI and CCSD(T)[43]. These simulations are critical in understanding supramolecular interactions, which are essential in biological and chemical systems[14]. The integration of quantum simulations into drug discovery offers several advantages. Firstly, it enables the accurate prediction of molecular properties, such as binding energies and reaction barriers, which are crucial for identifying promising drug candidates[24]. Secondly, quantum simulations can facilitate personalized medicine by analyzing complex molecular interactions specific to individual patients, allowing for tailored treatments[17]. Lastly, these simulations can reduce the reliance on empirical methods and enhance the efficiency of drug development pipelines, making life-saving medications more accessible and affordable[4]. Despite the current limitations of quantum hardware, ongoing research is focused on improving the accuracy and efficiency of quantum simulations[25]. Techniques such as quantum subspace expansions and orbital relaxations have been developed to achieve high accuracy without additional qubits or quantum operations. These advancements highlight the potential of quantum simulations to drive breakthroughs in drug discovery by providing unprecedented insights into molecular behavior[27,17].

Structure-Based Drug Design:

Structure-based drug design is a critical approach in pharmaceutical research that relies on understanding the three-dimensional structure of a target protein to design drugs that can bind effectively[44]. Quantum computing plays a pivotal role in enhancing this process by predicting binding affinities and optimizing drug candidates more accurately than classical methods[42]. Traditional computational methods, such as molecular dynamics and density functional theory (DFT), face limitations in accurately modeling complex molecular interactions due to computational constraints and the need for empirical approximations[45]. Quantum computing leverages quantum algorithms like the Variational Quantum Eigensolver (VQE) to simulate molecular systems with unprecedented accuracy[37]. VQE is particularly useful in calculating the electronic structure of molecules, which is essential for predicting binding affinities between drugs and their targets[29]. By accurately determining the ground-state energy of molecular systems, VQE can help identify the most stable conformations of drug candidates and their interactions with proteins, thereby optimizing drug design[31]. In structure-based drug design, the target protein's structure is a crucial input. Quantum simulations can enhance this process by providing detailed insights into protein-ligand interactions at the atomic level[30]. This allows researchers to predict how drug candidates will bind to specific sites on the protein, enabling the design of drugs with higher affinity and specificity[16]. Quantum machine learning algorithms can further accelerate this process by efficiently exploring vast chemical spaces to identify promising drug candidates and predict their properties and interactions with targets[46]. Quantum computing also facilitates molecular docking, a technique used to predict the preferred orientation of one molecule to a second when bound to each other[2]. By integrating quantum mechanics into molecular docking, researchers can improve the accuracy of binding affinity predictions, which is critical for identifying effective drug candidates[10]. Additionally, quantum simulations can enhance de novo design by simulating chemical pathways and predicting the synthesizability of drug candidates, thereby increasing the efficiency of new drug creation[11]. Despite the current limitations of quantum hardware, ongoing research is focused on developing hybrid quantum-classical workflows that can be applied to real-world drug design problems[38]. For instance, studies have developed pipelines that combine quantum simulations with classical optimization techniques to address challenges like covalent bond interactions and prodrug activation[19]. These advancements highlight the potential of quantum computing to drive breakthroughs in drug discovery by providing unprecedented insights into molecular behavior and interactions[47].

Target-Based Drug Discovery:

Target-based drug discovery is a pivotal approach in pharmaceutical research, focusing on identifying and validating specific biological targets for therapeutic intervention[36]. Quantum computing plays a transformative role in this process by enhancing target identification, validation, and lead optimization through its unparalleled computational capabilities[16]. Traditional methods often rely on empirical screening and classical computational tools, which can be time-consuming and less accurate in predicting molecular interactions[48]. Quantum computing leverages quantum algorithms like the Variational Quantum Eigensolver (VQE) to simulate molecular systems with unprecedented accuracy, providing insights into binding affinities and specificity[27]. This capability is particularly valuable for identifying "undruggable" targets, such as proteins with complex structures that lack clear binding sites[14]. By accurately determining the electronic structure of molecules, quantum simulations can help identify the most stable conformations of drug candidates and their interactions with proteins, thereby optimizing drug design[29]. In the context of target validation, quantum computing can enhance our understanding of drug-target interactions through quantum mechanics/molecular mechanics (QM/MM) simulations, which are critical for predicting the efficacy and safety of drug candidates[49]. Additionally, quantum machine learning algorithms can efficiently explore vast chemical spaces to identify promising drug candidates and predict their properties and interactions with targets[24]. Hybrid quantum-classical approaches are being developed to address real-world drug discovery challenges, such as simulating covalent bond interactions and predicting Gibbs free energy profiles for prodrug activation[14]. These advancements highlight the potential of quantum computing to drive breakthroughs in drug discovery by providing unprecedented insights into molecular behavior and interactions[21]. As quantum technology continues to evolve, it is expected to play a pivotal role in transforming the pharmaceutical industry, enabling faster, more accurate, and personalized drug discovery that can address complex health challenges more effectively than ever before[22]. The integration of quantum computing into drug development pipelines will not only benefit pharmaceutical companies by reducing costs and improving success rates but also contribute to societal well-being by making life-saving medications more accessible and affordable[28]. Furthermore, quantum computing can facilitate the optimization of lead compounds by accurately predicting their binding affinities and specificity, allowing researchers to refine their designs more efficiently[50]. This capability is crucial for enhancing the efficacy and safety of drugs, ultimately leading to better health outcomes and improved quality of life for patients globally[44,37].

Ligand-Based Drug Discovery:

Ligand-based drug discovery is a critical approach in pharmaceutical research that focuses on designing drugs based on their chemical properties rather than the three-dimensional structure of the target protein[16]. Quantum computing plays a transformative role in this process by predicting drug molecule designs without requiring detailed structural information. Traditional ligand-based methods often rely on quantitative structure-activity relationship (QSAR) models, which correlate chemical descriptors with biological activity[36],[47]. However, these models can be limited by their reliance on empirical data and classical computational methods[31]. Quantum computing offers a revolutionary alternative by leveraging quantum mechanical descriptors, which can be more precise and have higher predictive power[43,29]. These descriptors are derived from quantum simulations that capture the electronic structure of molecules, enabling the prediction of properties such as molecular stability, reactivity, and binding affinity[51]. Quantum algorithms can efficiently calculate these descriptors, providing a robust foundation for QSAR models[25,40]. This approach is particularly valuable when structural information about the target protein is unavailable or incomplete, allowing researchers to design drugs based on their chemical properties alone[52]. Quantum machine learning algorithms can further enhance this process by analyzing vast chemical spaces to identify promising drug candidates and predict their interactions with biological targets[24]. The integration of quantum computing into ligand-based drug discovery not only accelerates the identification of potential drugs but also enhances the accuracy of predictions, leading to more effective and safer treatments[43]. Additionally, quantum computing can facilitate the design of drugs with improved pharmacokinetic properties, such as solubility and bioavailability, by simulating molecular interactions in various environments[26]. As quantum technology continues to evolve, it is expected to play a pivotal role in transforming the pharmaceutical industry by enabling faster, more accurate, and personalized drug discovery that can address complex health challenges more effectively than ever before[46]. The potential of quantum computing to democratize drug discovery by making it more accessible and cost-effective is substantial, offering new opportunities for the development of safer and more effective treatments[32]. Furthermore, quantum computing can enhance our understanding of drug-target interactions through quantum mechanics/molecular mechanics (QM/MM) simulations, which are vital in the post-drug-design computational validation phase[53]. This development propels the field of computational drug development forward, enabling more precise predictions and optimizations in drug design[31]. Ultimately, the convergence of quantum computing and ligand-based drug discovery represents a groundbreaking opportunity to redefine the drug development process, promising a future where treatments are more effective, safer, and tailored to individual patient needs[42,38].

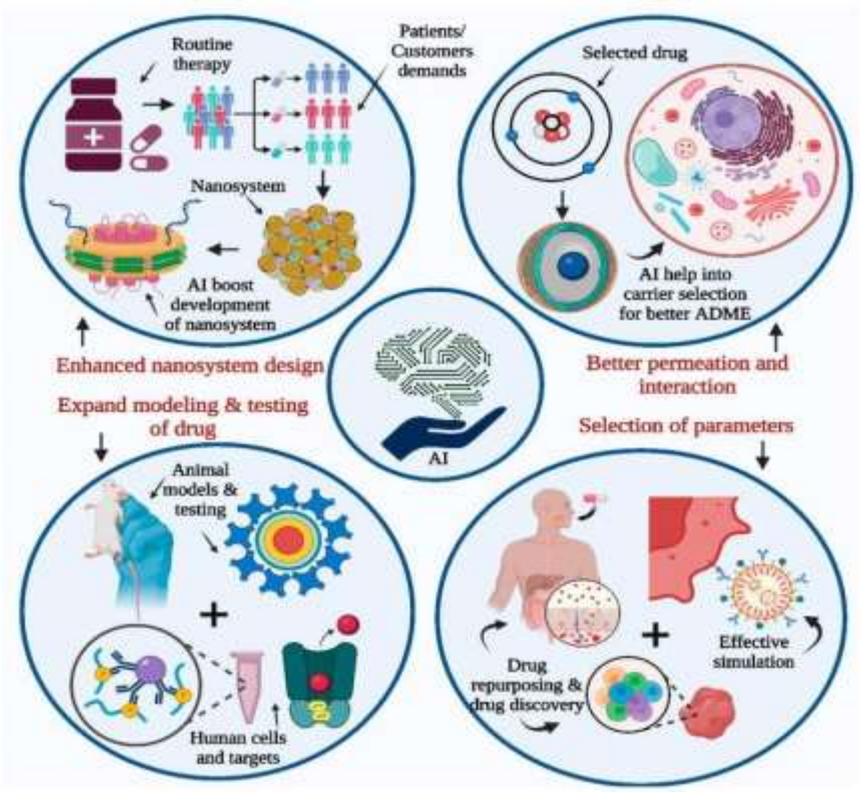

Figure.1 Role of Artificial Intelligence in Enhancing Drug Delivery through Nanosystems

Quantum AI in Personalized Medicine:
Quantum AI is revolutionizing personalized medicine by leveraging quantum computing to analyze vast genetic and clinical data, enabling the development of highly personalized treatment plans tailored to individual patient profiles[45]. This integration enhances predictive diagnostics and treatment customization, maximizing therapeutic efficacy while minimizing adverse effects through precise simulations and AI-driven insights[54].

Genomic Analysis:
Quantum AI is revolutionizing genomic analysis by leveraging quantum computing to analyze large-scale genomic data, enabling the tailoring of treatments to individual patients with unprecedented precision[24]. This integration combines the unparalleled computational power of quantum computing with the predictive capabilities of AI, allowing for the efficient processing of vast datasets that are beyond the capabilities of classical computers[55]. Quantum algorithms can analyze large-scale genomic and proteomic data sets with unprecedented speed, enabling the identification of genetic markers associated with disease susceptibility, drug response, and treatment outcomes[48]. By integrating quantum computing with advanced statistical methods, personalized medicine approaches can tailor treatment strategies to individual patients based on their unique genetic profiles, optimizing therapeutic efficacy and minimizing adverse reactions[36]. For instance, quantum machine learning models can predict how a patient will respond to specific therapies by analyzing large datasets of patient histories, genetic profiles, and treatment responses[51]. This capability not only increases the speed of computation but also

enhances the accuracy of medical decision-making, paving the way for more sophisticated diagnostic tools and predictive systems in healthcare[28]. Additionally, quantum-enhanced algorithms can uncover hidden patterns in genetic data, enabling the identification of biomarkers and the development of personalized treatment plans[46]. Quantum computing also accelerates whole-genome sequencing and mutation analysis, providing insights into genetic variations that influence drug response and disease susceptibility[29]. This capability is crucial for developing more effective and personalized treatment plans, reducing trial-and-error in prescribing medications and improving patient outcomes[30]. Furthermore, quantum cryptography provides robust solutions for secure storage and transmission of sensitive medical data, ensuring patient privacy and confidentiality in personalized medicine initiatives[21]. As quantum technology continues to evolve, it is expected to play a pivotal role in transforming healthcare by enabling faster, more accurate, and personalized medical treatments that can address complex health challenges more effectively than ever before[49]. Ultimately, the convergence of quantum AI and genomic analysis represents a groundbreaking opportunity to redefine healthcare, promising a future where treatments are more effective, safer, and tailored to individual patient needs, thereby revolutionizing healthcare outcomes worldwide[56].

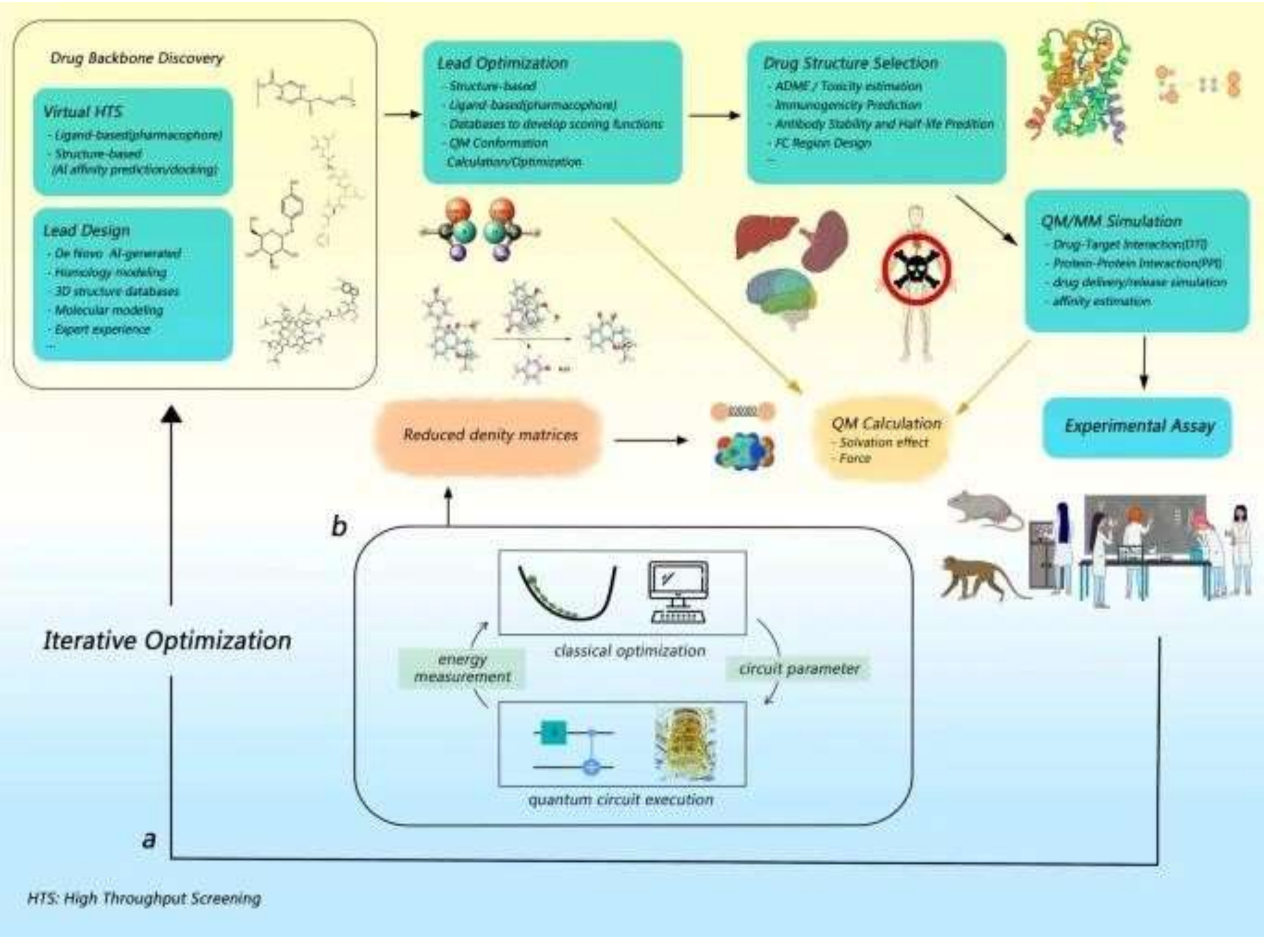

Figure2: Integration of Quantum and Classical Computing in Drug Discovery and Optimization

Quantum Bioinformatics:

The integration of quantum computing with bioinformatics is transforming personalized medicine by enhancing the analysis and interpretation of complex biological data[57]. Quantum computing leverages principles like superposition and entanglement to process vast amounts of data exponentially faster than classical computers, making it ideal for tasks such as genomic analysis and protein structure prediction[3]. In personalized medicine, this capability is crucial for tailoring treatments to individual patients based on their unique genetic profiles[58]. Quantum algorithms can rapidly analyze large-scale genomic data, identifying genetic markers associated with disease susceptibility and drug response, which is essential for developing personalized treatment plans[59]. For instance, quantum machine learning models can decipher complex genetic patterns and interactions that influence a patient's response to medications, allowing clinicians to prescribe drugs that are most likely to be effective while minimizing adverse effects[46]. The integration of quantum computing with existing bioinformatics tools, such as sequence alignment algorithms, can significantly improve efficiency and accuracy in analyzing genomic data[31]. Quantum-enhanced variant calling can quickly identify genetic mutations that influence an individual's response to certain medications, leading to more effective and personalized treatment plans[60]. Additionally, quantum algorithms can simulate complex biological systems, such as protein folding, which is vital for understanding disease mechanisms and designing targeted therapies[54]. This integration not only accelerates the discovery of new drugs by simulating molecular interactions at a scale that classical systems cannot handle efficiently but also optimizes clinical decision-making processes, leading to more precise diagnoses and treatment recommendations[10]. As quantum technology continues to evolve, it is expected to play a pivotal role in transforming healthcare by enabling faster, more accurate, and personalized medical treatments that can address complex health challenges more effectively than ever before[61]. Ultimately, the synergy between quantum computing and bioinformatics represents a groundbreaking opportunity to redefine personalized medicine, promising a future where treatments are more effective, safer, and tailored to individual patient needs, thereby revolutionizing healthcare outcomes worldwide[46],[62].

Table 1: Applications of AI and Quantum Computing Models in Drug Discovery and Design

Sr.no.	AI/Quantum model	Aim /target	Application	Benefits /impact	References
1	Hybrid Quantum Computing Pipeline	Precise molecular modeling and predictive analytics	Drug discovery, molecular interactions simulation	Enhances accuracy and efficiency in drug design	[4]
2	Gaussian Boson Sampling Light Quantum Processor (Abacus)	Molecular docking and RNA folding prediction	Drug design methods, high-throughput screening	Accelerates drug development by simulating complex biological systems	[32]
3	Quantum Mechanics/Molecular Mechanics (QM/MM) Simulations	Understanding drug-target interactions	Post-drug-design computational validation	Provides detailed insights into covalent inhibitors	[62,53]
4	Neutral-Atom Quantum Computer (Orion)	Protein hydration analysis and ligand-protein binding studies	Molecular biology tasks, drug discovery	Revolutionizes computational drug discovery by accurately modeling water molecules in protein pockets	[59]
5	Variational Quantum Eigensolver (VQE)	Improving classical methods like Hartree-Fock	Quantum chemical calculations, drug design	Offers more accurate solutions for complex molecular systems	[43]
6	Quantum Computing Enhanced CADD	Predicting molecular properties with high accuracy	Computer-assisted drug discovery, screening drug candidates	Increases the scope of biological mechanisms and shortens screening time	[39]
7	Machine Learning (ML) Algorithms	Uncovering new structure-property relationships	Hypothesis generation and validation in drug discovery	Enables automated drug discovery approaches	[27]

8	Quantum Systems for Molecular Stability	Calculating molecular stability, binding affinity, and toxicity	Identifying promising drug candidates	More efficient than classical methods	[65],[17]
9	Quantum Computing for Protein Folding	Modeling protein folding and interactions	Drug candidate screening against multiple target structures	Allows parallel screening of drug candidates	[54],[63]
10	Hybrid Quantum-Classical Approach	Analyzing protein hydration and ligand binding	Enhancing drug design accuracy and efficiency	Combines classical and quantum algorithms for precise water molecule placement	[34]
11	Quantum Computing for High-Dimensional Problems	Addressing complex molecular interactions	Accelerating drug discovery and development	Enables faster and more accurate simulation of molecular interactions	[38]
12	Simulation-Based Drug Discovery	Moving beyond digitally enabled R&D to in silico drug discoveries	Pharmaceutical R&D, drug development cycle optimization	Could trigger a paradigm shift in pharmaceutical research	[58]

Challenges and Limitations:

Quantum computing faces significant challenges, including the limitations of noisy intermediate-scale quantum (NISQ) devices, which are prone to errors due to quantum noise and lack the scalability needed for large-scale computations[32]. Addressing these challenges requires advancements in quantum error correction and hardware development to achieve fault-tolerant quantum computing capable of solving complex problems efficiently[5].

Current State of Quantum Computing:

The current state of quantum computing is dominated by noisy intermediate-scale quantum (NISQ) devices, which are characterized by their limited number of qubits and high error rates. NISQ devices typically range from tens to a few hundred qubits and are subject to significant levels of quantum noise and errors, making them unsuitable for large-scale, fault-tolerant quantum computations[62]. The primary limitations of NISQ devices include their inability to perform full quantum error correction, limited qubit coherence, and noisy operations, which lead to errors in quantum gate operations and measurements[63]. These errors accumulate quickly, limiting the depth of quantum circuits that can be executed reliably, and often result in inconsistent results due to device instability[46]. Despite these challenges, NISQ devices are being used for practical applications such as quantum machine learning, optimization problems, and quantum simulations, leveraging algorithms like the Variational Quantum Eigensolver (VQE) and Quantum Approximate Optimization Algorithm (QAOA)[28]. These algorithms often involve hybrid quantum-classical approaches to compensate for the limitations of NISQ devices by leveraging classical computing resources. The NISQ era is seen as a transitional phase toward more powerful, fault-tolerant quantum computers, with ongoing research focused on improving qubit quality, developing noise-resilient algorithms, and understanding the propagation of errors in entangled systems[53]. While NISQ devices can demonstrate quantum advantages in specific tasks, such as quantum supremacy demonstrations, they are unlikely to outperform classical computers in many practical problems due to their noise levels[47]. The development of fault-tolerant quantum computing will require significant advancements in quantum error correction and scalability, which are crucial for realizing the full potential of quantum algorithms and applications[63]. As quantum technology continues to evolve, the lessons learned from NISQ devices will inform the development of future generations of quantum computers, paving the way toward more robust and reliable systems capable of solving complex problems efficiently[64]. Ultimately, the future of quantum computing depends on overcoming the limitations of NISQ devices and developing scalable, reliable systems that can be applied to real-world problems, leading to breakthroughs in fields like medicine, finance, and cybersecurity[65].

Error Correction and Scalability:

Error correction and scalability are two of the most significant challenges facing quantum computing as it transitions from theoretical concepts to practical applications[66]. Quantum error correction is essential for large-scale quantum systems because qubits are highly susceptible to decoherence, which leads to a loss of quantum information due to interactions with the environment[67]. Unlike classical bits, qubits can suffer from both bit flip errors (where a 0 becomes a 1 or vice versa) and phase flip errors, complicating error correction[68]. The no-cloning theorem further complicates matters by preventing the creation of perfect copies of qubit states, which is a common strategy in classical error correction[69]. Quantum error correction codes, such as surface codes, address these challenges by distributing quantum information across multiple qubits, allowing errors to be detected and corrected without disturbing the encoded state[70]. However, implementing these codes requires significant hardware overhead, including additional qubits and quantum gates, which can introduce more opportunities for errors[71]. Scaling up quantum computing to achieve fault-tolerant operations is another major challenge. Currently, most quantum devices are noisy intermediate-scale quantum (NISQ) devices, which are limited by their high error rates and inability to perform full quantum error correction[65]. Achieving fault-tolerant quantum computing requires reducing the physical error rate of qubits below a certain threshold, known as the error correction threshold[47]. Recent advancements, such as the demonstration of below-threshold error correction by Google using their Willow chip, signal progress toward overcoming these challenges[53]. However, scaling to millions of qubits while maintaining low error rates is a daunting task that requires significant advancements in both hardware and software[24]. The development of robust quantum error correction techniques is crucial for unlocking the full potential of quantum computing, enabling the execution of complex algorithms like Shor's algorithm and qubitization for quantum simulation[22]. As quantum technology continues to evolve, addressing these challenges will be pivotal for transforming various industries by providing unprecedented computational power and efficiency, leading to breakthroughs in fields like medicine, finance, and cybersecurity[34]. Ultimately, the future of quantum computing depends on overcoming the limitations of current devices and developing scalable, reliable systems that can be applied to real-world problems, leading to significant advancements in computational capabilities and practical applications[53].

Future Directions and Potential Impact:

Quantum AI, a synergy of quantum computing and artificial intelligence, is poised to revolutionize the pharmaceutical industry by accelerating drug development and leading to groundbreaking discoveries[72]. This integration combines the unparalleled computational power of quantum computing with the predictive capabilities of AI, enabling the solution of complex problems more efficiently than ever before[73]. Quantum AI can significantly reduce the time and cost of bringing new drugs to market by enhancing the accuracy and speed of molecular modeling and simulation, crucial for understanding drug-target interactions and optimizing drug candidates[71]. Traditional drug development processes are often time-consuming and costly, involving extensive experimentation and trial-and-error approaches[62]. Quantum AI offers a transformative solution by leveraging quantum algorithms like the Variational Quantum Eigensolver (VQE) to simulate complex molecular systems with unprecedented accuracy, predicting binding affinities and pharmacokinetic properties more effectively than classical methods[74]. For instance, researchers at the University of Toronto have demonstrated the potential of quantum computing to accelerate the early stages of drug discovery by identifying molecules that interact with the "undruggable" KRAS protein, a common target in cancer research[75]. This capability significantly reduces the time required for preclinical testing, allowing promising drug candidates to reach clinical trials faster[7]. Additionally, AI-driven generative models can design new molecules with optimized properties, further streamlining the drug discovery process[54]. By integrating quantum computing into AI-driven pipelines, pharmaceutical companies can accelerate the identification of promising drug candidates, optimize their pharmacokinetic properties, and predict potential side effects more accurately, leading to safer and more effective treatments[64].

The potential for Quantum AI to lead to groundbreaking discoveries in pharmaceuticals is substantial[53]. By simulating complex molecular interactions that are beyond the capabilities of classical computers, Quantum AI can uncover new drug targets and mechanisms of action that were previously inaccessible[47]. This capability is particularly promising for addressing "undruggable" targets, such as the KRAS protein, which has been challenging to target effectively with traditional methods[62]. Quantum AI can also enhance our understanding of drug-target interactions through quantum mechanics/molecular mechanics (QM/MM) simulations, which are vital in the post-drug-design computational validation phase[38]. This development not only facilitates a detailed examination of covalent inhibitors but also propels the field of computational drug development forward[42]. Furthermore, Quantum AI can facilitate the creation of new types of drug-candidate libraries that are no longer restricted to small molecules but also include peptides and antibodies, allowing for a more automated approach to drug discovery[73]. Additionally, quantum simulations can enhance our understanding of drug-target interactions, enabling the design of drugs with higher affinity and specificity[26]. This capability is crucial for developing more effective treatments for complex diseases, where traditional drugs often have limited efficacy or significant side effects. The integration of Quantum AI into pharmaceutical research also underscores the importance of interdisciplinary

collaboration between quantum physicists, AI researchers, and pharmaceutical scientists to fully harness its potential[42]. Despite the challenges associated with implementing Quantum AI in legacy systems and addressing ethical considerations, the long-term benefits are substantial, positioning early adopters for significant competitive advantages in the future[31]. As the technology matures, it is crucial for stakeholders to invest in research and development, ensuring that Quantum AI is harnessed responsibly and effectively to transform the pharmaceutical landscape[74]. By embracing this cutting-edge technology, the pharmaceutical industry can embark on a new era of innovation, where drug discovery is faster, more precise, and more patient-centric than ever before[16]. Ultimately, the convergence of Quantum AI and pharmaceuticals represents a groundbreaking opportunity to redefine the drug development process, promising a future where treatments are more effective, safer, and tailored to individual patient needs, thereby revolutionizing healthcare outcomes worldwide[49].
Quantum AI also has the potential to disrupt traditional drug discovery methods by providing a more efficient and cost-effective approach[62]. For example, Pfizer has collaborated with XtalPi to leverage quantum physics and AI in predicting the 3D structure of molecules, significantly reducing the time required for crystal structure prediction from months to days[70]. This capability not only accelerates the early stages of drug discovery but also enhances the accuracy of predictions, allowing researchers to focus on the most promising candidates[58]. Additionally, AI and quantum computing can accelerate drug discovery by enabling significant savings on the resources needed to test compounds, thereby reducing development costs and improving drug approval rates[76]. As Quantum AI continues to evolve, it is expected to play a pivotal role in transforming the pharmaceutical industry, enabling faster, more accurate, and personalized drug discovery that can address complex health challenges more effectively than ever before[59]. The integration of Quantum AI into drug development pipelines will not only benefit pharmaceutical companies by reducing costs and improving success rates but also contribute to societal well-being by making life-saving medications more accessible and affordable[70]. Furthermore, Quantum AI can facilitate personalized medicine by analyzing vast amounts of patient data to tailor treatments to individual needs, enhancing treatment efficacy and patient adherence[68]. This personalized approach not only improves patient outcomes but also reduces healthcare costs by minimizing ineffective treatments[50]. Ultimately, the future of drug discovery and development will be shaped by the synergy between AI and quantum computing, leading to breakthroughs in treating complex diseases and improving healthcare outcomes globally[65,73].

Conclusion:

The convergence of quantum computing and artificial intelligence, termed Quantum AI, heralds a transformative era for pharmaceutical drug design, offering solutions to longstanding challenges in efficiency, accuracy, and personalization. By harnessing quantum principles such as superposition, entanglement, and interference, Quantum AI enables unprecedented computational power, surpassing classical methods like Density Functional Theory. Algorithms like the Variational Quantum Eigensolver and Quantum Phase Estimation facilitate precise molecular simulations, optimizing drug-target interactions and expanding drug-candidate libraries to include peptides and antibodies. This technology accelerates the identification of promising candidates, enhances pharmacokinetic predictions, and reduces reliance on costly empirical approaches, potentially lowering development costs and timeframes. Furthermore, Quantum AI's ability to analyze vast genomic datasets drives personalized medicine, tailoring treatments to individual genetic profiles for improved efficacy and safety. Despite current limitations, such as noisy intermediate-scale quantum devices and the need for robust error correction, ongoing advancements in quantum hardware and algorithms signal a promising future. Interdisciplinary collaboration among quantum physicists, AI researchers, and pharmaceutical scientists is crucial to overcoming these hurdles and fully realizing Quantum AI's potential. As the technology matures, it is poised to redefine drug discovery, making it more simulation-driven, cost-effective, and patient-centric. This paradigm shift promises not only competitive advantages for early adopters but also societal benefits through accessible, life-saving medications, ultimately revolutionizing healthcare outcomes worldwide.

REFERENCES

1. P. Hassanzadeh, F. Atyabi, and R. Dinarvand, "The significance of artificial intelligence in drug delivery system design," *Adv. Drug Deliv. Rev.*, vol. 151–152, pp. 169–190, 2019, doi: 10.1016/j.addr.2019.05.001.
2. V. Chavda et al., *Bioinformatics Tools for Pharmaceutical Drug Product Development*. Hoboken, NJ, USA: John Wiley & Sons, Ltd., 2023, pp. 117–145.
3. G. M. Sacha and P. Varona, "Artificial intelligence in nanotechnology," *Nanotechnology*, vol. 24, p. 452002, 2013, doi: 10.1088/0957-4484/24/45/452002.
4. W. Wong, E. Chee, J. Li, and X. Wang, "Recurrent neural network-based model predictive control for continuous pharmaceutical manufacturing," *Mathematics*, vol. 6, p. 242, 2018, doi: 10.3390/math6110242.
5. J. Wise et al., "The positive impacts of real-world data on the challenges facing the evolution of biopharma," *Drug Discov. Today*, vol. 23, pp. 788–801, 2018, doi: 10.1016/j.drudis.2018.01.034.
6. D. Taylor, S. G. Bowden, R. Knorr, D. R. Wilson, J. Proudfoot, and A. E. Dunlop, "The Pistoia Alliance controlled substance compliance service project: From start to finish," *Drug Discov. Today*, vol. 20, pp. 175–180, 2015, doi: 10.1016/j.drudis.2014.09.021.

7. C. K. H. Lee, K. L. Choy, and Y. N. Chan, “A knowledge-based ingredient formulation system for chemical product development in the personal care industry,” *Comput. Chem. Eng.*, vol. 65, pp. 40–53, 2014, doi: 10.1016/j.compchemeng.2014.03.004.
8. J. Schmidhuber, “Deep learning in neural networks: An overview,” *Neural Netw.*, vol. 61, pp. 85–117, 2015, doi: 10.1016/j.neunet.2014.09.003.
9. I. H. Sarker, “Machine learning: Algorithms, real-world applications and research directions,” *SN Comput. Sci.*, vol. 2, p. 160, 2021, doi: 10.1007/s42979-021-00592-x.
10. I. H. Sarker, “AI-based modeling: Techniques, applications and research issues towards automation, intelligent and smart systems,” *SN Comput. Sci.*, vol. 3, p. 158, 2022, doi: 10.1007/s42979-022-01043-x.
11. S. Dara, S. Dhamercherla, S. S. Jadav, C. M. Babu, and M. J. Ahsan, “Machine learning in drug discovery: A review,” *Artif. Intell. Rev.*, vol. 55, pp. 1947–1999, 2022, doi: 10.1007/s10462-021-10058-4.
12. I. Kavasidis et al., “Predictive maintenance in pharmaceutical manufacturing lines using deep transformers,” *Procedia Comput. Sci.*, vol. 220, pp. 576–583, 2023, doi: 10.1016/j.procs.2023.03.073.
13. I. Adzhubei et al., “Predicting functional effect of human missense mutations using PolyPhen-2,” *Curr. Protoc. Hum. Genet.*, vol. Chapter 7, Unit7.20, 2013.
14. W. Alvarado et al., “Understanding the enzyme–ligand complex: Insights from all-atom simulations of butyrylcholinesterase inhibition,” *J. Biomol. Struct. Dyn.*, vol. 38, pp. 1028–1041, 2020.
15. O. A. Arodola et al., “Quantum mechanics implementation in drug-design workflows: Does it really help?” *Drug Des. Devel. Ther.*, vol. 11, pp. 2551–2564, 2017.
16. P. Ball, “First quantum computer to pack 100 qubits enters crowded race,” *Nature*, vol. 599, p. 542, 2021.
17. L. Banchi et al., “Molecular docking with Gaussian Boson Sampling,” *Sci. Adv.*, vol. 6, p. eaax1950, 2020.
18. P. R. Batista et al., “Molecular dynamics simulations applied to the study of subtypes of HIV-1 protease,” *Cell Biochem. Biophys.*, vol. 44, pp. 395–404, 2006.
19. H. J. C. Berendsen et al., “GROMACS: A message-passing parallel molecular dynamics implementation,” *Comput. Phys. Commun.*, vol. 91, pp. 43–56, 1995.
20. V. Bergholm et al., “PennyLane: Automatic differentiation of hybrid quantum-classical computations,” *arXiv preprint*, 2018.
21. M. Berry et al., “Potential broad-spectrum inhibitors of the coronavirus 3CLpro: A virtual screening and structure-based drug design study,” *Viruses*, vol. 7, pp. 6642–6660, 2015.
22. P. L. Bremer et al., “Overcoming the heuristic nature of k-means clustering: Identification and characterization of binding modes from simulations of molecular recognition complexes,” *J. Chem. Inf. Model.*, vol. 60, pp. 3081–3092, 2020.
23. Y. Cao et al., "Potential of quantum computing for drug discovery," *IBM J. Res. Dev.*, vol. 62, no. 6, pp. 6:1–6:20, 2018.
24. K. Choo et al., "Fermionic neural-network states for ab-initio electronic structure," *Nat. Commun.*, vol. 11, p. 2368, 2020.
25. E. V. Davydov et al., "Identifying a high fraction of the human genome to be under selective constraint using GERP++," *PLoS Comput. Biol.*, vol. 6, p. e1001025, 2010.
26. Y. Duan et al., "A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations," *J. Comput. Chem.*, vol. 24, pp. 1999–2012, 2003.
27. A. Dunham et al., "A missense variant effect prediction and annotation resource for SARS-CoV-2," *bioRxiv* preprint, 2021, doi: 10.1101/2021.02.24.432721.
28. P. S. Emani et al., "Quantum computing at the frontiers of biological sciences," *Nat. Methods*, vol. 18, pp. 701–709, 2021.
29. E. Farhi et al., "Classification with quantum neural networks on near term processors," *arXiv* preprint:1802.06002v2, 2018.
30. R. P. Feynman, "Simulating physics with computers," *Int. J. Theor. Phys.*, vol. 21, pp. 467–488, 1982.
31. D. M. Fox et al., "mRNA codon optimization with quantum computers," *PLoS One*, vol. 16, p. e0259101, 2021.
32. V. Giovannetti et al., "Quantum random access memory," *Phys. Rev. Lett.*, vol. 100, p. 160501, 2008.
33. B. Hess et al., "GROMACS 4: algorithms for highly efficient, load-balanced, and scalable molecular simulation," *J. Chem. Theory Comput.*, vol. 4, pp. 435–447, 2008.
34. W. D. Jang et al., "Drugs repurposed for COVID-19 by virtual screening of 6,218 drugs and cell-based assay," *Proc. Natl. Acad. Sci. USA*, vol. 118, p. e2024302118, 2021.
35. M. H. Khatami et al., "Gate-based quantum computing for protein design," *arXiv* preprint:2201.12459, 2022.
36. P. Kumar et al., "Predicting the effects of coding non-synonymous variants on protein function using the SIFT algorithm," *Nat. Protoc.*, vol. 4, pp. 1073–1081, 2009.
37. C. C. Lee et al., "Structural basis of inhibition specificities of 3C and 3C-like proteases by zinc-coordinating and peptidomimetic compounds," *J. Biol. Chem.*, vol. 284, pp. 7646–7655, 2009.

38. A. Blanco-González, A. Cabezón, D. Seco-González, P. Conde-Torres, Á. Antelo-Riveiro, et al., "The role of AI in drug discovery: Challenges, opportunities, and strategies," *Pharmaceuticals*, vol. 16, no. 6, p. 891, Jun. 2023.
39. K. Arute, R. Arya, D. Babbush, D. Bacon, and J. C. Bardin, "Quantum supremacy using a programmable superconducting processor," *Nature*, vol. 574, no. 7779, pp. 505–510, Oct. 2019.
40. M. Zinner, F. Dahlhausen, P. Boehme, J. Ehlers, L. Bieske, and L. Fehring, "Quantum computing's potential for drug discovery: Early stage industry dynamics," *Drug Discovery Today*, vol. 26, no. 7, pp. 1680–1688, Jul. 2021.
41. A. Biswas, A. Basu, A. Nandy, A. Deb, K. Haque, and D. Chanda, "Drug discovery and drug identification using AI," in *Proc. Indo–Taiwan 2nd Int. Conf. Comput. Anal. Netw. (Indo-Taiwan ICAN)*, pp. 49–51, Feb. 2020.
42. M. D. Parenti and G. Rastelli, "Advances and applications of binding affinity prediction methods in drug discovery," *Biotechnol. Adv.*, vol. 30, no. 1, pp. 244–250, Jan. 2012.
43. J. Li, R. O. Topaloglu, and S. Ghosh, "Quantum generative models for small molecule drug discovery," *IEEE Trans. Quantum Eng.*, vol. 2, pp. 1–8, 2021.
44. V. Chauhan, S. Negi, D. Jain, P. Singh, A. K. Sagar, and A. K. Sharma, "Quantum computers: A review on how quantum computing can boom AI," in *Proc. 2nd Int. Conf. Advance Comput. Innov. Technol. Eng. (ICACITE)*, pp. 559–563, Apr. 2022.
45. S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin, and X. Yuan, "Quantum computational chemistry," *Rev. Mod. Phys.*, vol. 92, Mar. 2020.
46. S. Duela, A. Umamageswari, R. Prabavathi, P. Umapathy, and K. Raja, "Quantum assisted genetic algorithm for sequencing compatible amino acids in drug design," in *Proc. 3rd Int. Conf. Adv. Electr. Comput. Commun. Sustain. Technol. (ICAECT)*, pp. 1–7, Jan. 2023.
47. B. Lau, P. S. Emani, J. Chapman, L. Yao, T. Lam, P. Merrill, et al., "Insights from incorporating quantum computing into drug design workflows," *Bioinformatics*, vol. 39, no. 1, Jan. 2023.
48. H. Mustafa, S. N. Morapakula, P. Jain, and S. Ganguly, "Variational quantum algorithms for chemical simulation and drug discovery," in *Proc. Int. Conf. Trends Quantum Comput. Emerg. Bus. Technol. (TQCEBT)*, pp. 1–8, Oct. 2022.
49. O. Dupouët, Y. Pitarch, M. Ferru, and B. Bernela, "Community dynamics and knowledge production: Forty years of research in quantum computing," *J. Knowl. Manage.*, vol. 28, no. 3, pp. 651–672, 2024.
50. Y. Cao, J. Romero, and A. Aspuru-Guzik, "Potential of quantum computing for drug discovery," *IBM J. Res. Develop.*, vol. 62, no. 6, Nov. 2018.
51. J. Singh and M. Singh, "Evolution in quantum computing," in *Proc. Int. Conf. Syst. Model. Advancement Res. Trends (SMART)*, Nov. 2016, pp. 267–270.
52. S. K. Sood and Pooja, "Quantum computing review: A decade of research," *IEEE Trans. Eng. Manag.*, vol. 71, pp. 6662–6676, 2024.
53. E. H. Shaik and N. Rangaswamy, "Implementation of quantum gates based logic circuits using IBM qiskit," in *Proc. 5th Int. Conf. Comput. Commun. Secur. (ICCCS)*, Oct. 2020, pp. 1–6.
54. C. Outeiral, M. Strahm, J. Shi, G. M. Morris, S. C. Benjamin, and C. M. Deane, "The prospects of quantum computing in computational molecular biology," *Wiley Interdiscip. Rev. Comput. Mol. Sci.*, vol. 11, p. e1481, 2021.
55. O. A. von Lilienfeld, K. R. Müller, and A. Tkatchenko, "Exploring chemical compound space with quantum-based machine learning," *Nat. Rev. Chem.*, vol. 4, pp. 347–358, 2020.
56. J. Singh and K. S. Bhangu, "Contemporary quantum computing use cases: Taxonomy, review and challenges," *Arch. Comput. Methods Eng.*, vol. 30, pp. 615–638, 2023.
57. B. A. Cordier, N. P. Sawaya, G. G. Guerreschi, and S. K. McWeeney, "Biology and medicine in the landscape of quantum advantages," *J. R. Soc. Interface*, vol. 19, p. 20220541, 2022.
58. L. Marchetti et al., "Quantum computing algorithms: Getting closer to critical problems in computational biology," *Brief. Bioinform.*, vol. 23, p. bbac437, 2022.
59. M. Sajjan et al., "Quantum machine learning for chemistry and physics," *Chem. Soc. Rev.*, vol. 51, pp. 6475–6573, 2022.
60. S. McArdle, S. Endo, A. Aspuru-Guzik, S. C. Benjamin, and X. Yuan, "Quantum computational chemistry," *Rev. Mod. Phys.*, vol. 92, p. 015003, 2020.
61. M. Avramouli, I. Savvas, A. Vasilaki, G. Garani, and A. Xenakis, "Quantum machine learning in drug discovery: Current state and challenges," in *Proc. 26th Pan-Hellenic Conf. Informatics*, Athens, Greece, Nov. 2022, pp. 394–401.
62. P. Carracedo-Reboredo et al., "A review on machine learning approaches and trends in drug discovery," *Comput. Struct. Biotechnol. J.*, vol. 19, pp. 4538–4558, 2021.
63. G. Sliwoski, S. Kothiwale, J. Meiler, and E. W. Lowe, "Computational methods in drug discovery," *Pharmacol. Res.*, vol. 66, pp. 334–395, 2014.
64. M. Zinner et al., "Quantum computing's potential for drug discovery: Early stage industry dynamics," *Drug Discov. Today*, vol. 26, pp. 1680–1688, 2021.

65. M. Zinner et al., "Toward the institutionalization of quantum computing in pharmaceutical research," *Drug Discov. Today*, vol. 27, pp. 378–383, 2022.
66. G. U. Vasanthakumar and M. Singh, "Quantum machine learning in healthcare: Diagnostics and drug discovery," in *Quantum Machine Learning: Quantum Algorithms and Neural Networks*, 2024, p. 39.
67. T. D. Ladd et al., "Quantum computers," *Nature*, vol. 464, no. 7285, pp. 45–53, 2010.
68. S. Bravyi et al., "The future of quantum computing with superconducting qubits," *J. Appl. Phys.*, vol. 132, no. 16, 2022.
69. W. Li, "Quantum-accelerated big data analytics on cloud platforms: Leveraging quantum computing for large-scale data processing," *J. Big-Data Analytics Cloud Comput.*, vol. 9, no. 1, pp. 14–24, 2024.
70. W. Li, Z. Yin, X. Li et al., "A hybrid quantum computing pipeline for real-world drug discovery," *Sci. Rep.*, vol. 14, no. 1, p. 16942, 2024.
71. W. R. Myers, "Potential applications of microtesla magnetic resonance imaging detected using a superconducting quantum interference device," 2006.
72. Y. Cao, J. Romero, and A. Aspuru-Guzik, "Potential of quantum computing for drug discovery," *IBM J. Res. Develop.*, vol. 62, no. 6, pp. 6:1–6:20, 2018.
73. P. Sharma, "Quantum computing in drug design: Enhancing precision and efficiency in pharmaceutical development," *Sage Sci. Rev. Appl. Mach. Learn.*, vol. 7, no. 1, pp. 1–9, 2024.
74. G. A. Pinheiro et al., "Machine learning prediction of nine molecular properties based on the SMILES representation of the QM9 quantum-chemistry dataset," *J. Phys. Chem. A*, vol. 124, no. 47, pp. 9854–9866, 2020.
75. R. Mishra et al., "Quantum computing and its promise in drug discovery," in *Drug Delivery Systems Using Quantum Computing*, 2024, pp. 57–92.
76. L. Marchetti et al., "Quantum computing algorithms: Getting closer to critical problems in computational biology," *Brief. Bioinform.*, vol. 23, no. 6, p. bbac437, 2022.