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Quantum Computing and Drug Discovery: Current Trends and Future

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ABSTRACT:
Discovery of drugs is one the time consuming and resource intensive process in the pharmaceutical industry since it takes years of research and investments. Discovery of new drugs is crucial for preserving human health and eradication of diseases. Modern drug discovery processes like CADD relies on Traditional Computing which is constrained by its raw computing power because it struggles to simulate complex interactions between biomolecules. Therefore, pharmaceutical industry can be one of the largest beneficiaries of quantum technology pushing boundaries of innovation. Quantum Computing can accelerate the drug discovery process and execute them within few minutes to hours which would require millions of years on today's fastest supercomputer.
This paper explains Quantum Computing basics, principles of quantum computing, algorithms used in quantum computing like Shor, Grover's etc., Process of traditional drug discovery, limitations of CADD, Quantum Simulations, Virtual Screening, Molecular Docking and how Quantum Technology speeds up drug discovery process. It also addresses challenges regarding quantum technologies such as regulatory compliances, hardware limitations, cost & accessibility etc. and provides recent breakthroughs that demonstrates the application of quantum computing in drug discovery. Note that some very important terminologies related to quantum computing which are not mentioned in detail are mentioned in brief in our glossary section.

Keywords: Quantum Computing, Molecular Docking, Virtual Screening, Drug Discovery, Quantum Simulation, QSAR, CADD, Graph Neural Networks (GNNs), VQE, QPE, Suzuki-Miyaura, KRAS.

1. Introduction

The Quantum Computing domain is attracting various researchers, due to its promising outcomes. Today, computers have become vital for businesses, scientific research or missions, students, educational institutions, consumers and others. This type computers are known as Classical Computers which operate on the principles of Classical Physics. These computers are capable of executing large amount of calculation in a far less time.
But there are come calculations that Classical Computers would take thousands of years to perform and would require a large number of bits, such as simulation on sub-atomic levels that would take a classical computer thousands of years. Thus, a new system of computing was proposed that would employ the principles of quantum mechanics to break similar problems more efficiently and snappily. therefore, born the field of Quantum Computing where complex problems would be solved in less time such as taking 200 seconds as compared to same on the fastest supercomputer that would take exponential time. A

Quantum Computer is a device that leverages the principles of Quantum Mechanics to carry out processing of the data or that works on principles of Quantum Physics. The idea of developing a computer based on Quantum Mechanics goes back to 1981, when Richard Feynman, a renowned Physicist, proposed simulating Quantum System with Quantum Computers.

Quantum Computer like Classical Computers store information in the form of q-bits that are quantum version of bits. In classical computers, a bit is a fundamental unit of storage that can be either 0 or 1. Classical bits can be only in one state at a time, either 1 or 0.Q-bits on the other hand, can be 1, 0 or a combination of both. This property of being in many states at the same time is known as Superposition. Thus, this gives various possibilities at a time making it ideal for deriving solutions for complex problems, which in case of classical computers are difficult to achieve. Because of this advantage over classical computer, various Firms like Google, Microsoft, IBM and others are investing heavily to develop a sophisticated quantum computers for a specific set of problems.

2. Literature Review

Several studies have explored the evolution of computational techniques in drug discovery, beginning with conventional Computer-Aided Drug Discovery (CADD) frameworks that rely on molecular docking, QSAR modelling, and virtual screening [11,16]. While these classical methods have successfully accelerated early-stage drug design, multiple reviews emphasize their limitations in scaling to complex and flexible biomolecules due to exponential growth in computational resources [12]. Molecular dynamics simulations (MDS) and density functional theory (DFT) offer higher accuracy but remain computationally expensive when applied to large protein–ligand systems, further motivating the transition toward quantum-enhanced models.

Recent survey works, such as those by Rajendran et al. [12] and Kumar et al. [21], provide foundational insight into quantum algorithms like Variational Quantum Eigen solver (VQE), Quantum Phase Estimation (QPE), and Grover's search in the context of pharmaceutical research. Parallel efforts in Quantum Machine Learning (QML) have demonstrated improved prediction accuracy in virtual screening tasks using hybrid quantum–classical neural networks [18,19]. However, existing literature primarily addresses either algorithmic development or hardware feasibility in isolation. In contrast, the present work consolidates these perspectives by integrating algorithmic foundations, current limitations, and real-world case studies from industry deployments, offering a holistic overview of the quantum revolution in drug discovery.

3. Principles of Quantum Computing

Quantum Computers work on four principles of Quantum Mechanics:

1**). Superposition:** This property states that a q-bit can be in multiple states at the same time like it could be 0, 1 or weighted combination of both. This state is intact unless there is some outside interference.

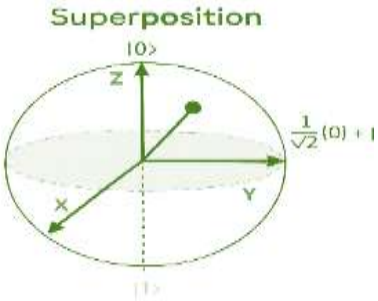

Figure 1:Superposition

2). **Entanglement:** Entanglement is the property that tells the correlation between qubits. The state of one qubit is influenced by the changes made in other no matter how far apart they are from each other.

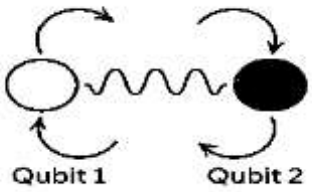

Figure 2: Two Entangled Qubits

3). Interference: Interference is the property that can alter the property of a qubit. Interference can be constructive or destructive and can be used to change the property of qubits or diminish their quantum state.

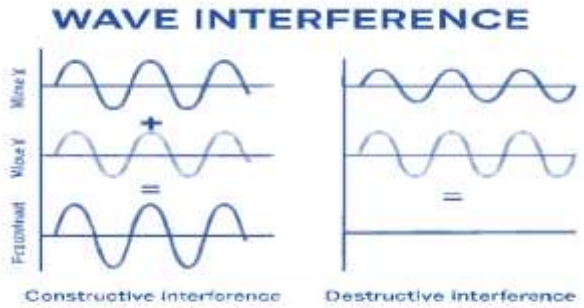

Figure 3: Interference

Constructive Interference can combine two waves therefore resulting in appending of properties while Destructive Interference can destroy the quantum state of a qubit thus, making them to be in a one position at a time.

4). Decoherence: Decoherence states the factors that would result in losing quantum state of a qubit and making it to behave like a normal bit. This is the biggest challenge in quantum computing. As stated earlier, qubits maintain their quantum state unless there is some external interference therefore, Quantum Computers are kept in a dilute refrigerator where the temperature is kept near to absolute zero, in order to maintain their quantum state. These principles of quantum computing are useful in specialized tasks such

as those of physical and chemical sciences and others like simulating atoms, weather forecasting, simulation to understand nature, machine learning etc.

4. Trends in Quantum Computing

Leading tech giants like Google, IBM, Amazon and startups like Rigetti and Ionq are funding this technology heavily. Quantum Computing is estimated to turn 1.35 trillion USD industry by 2035.[1]
Many Developments have happened over the years in this field. Some of them are discussed below:

1. **Majorana 1:** A new quantum chip unveiled by Microsoft in 2025 which encompasses topological architecture aiming to solve industrial scale problems within years instead of decades. It is also world's first topo-conductor chip that contains topo-conductor a material that allows observing and controlling particles of Majorana leading to production of reliable and scalable qubits (up to 1 million qubits) [2].
2. **Google's Willow Quantum Chip**: Google's Willow Chip reduces errors exponentially as more qubits are scaled up. According to Google it completed a given benchmark within 5 minutes that requires a fastest super- computer around 10 septillion years [3].
3. **IBM Osprey**: A 433-qubit quantum chip developed by IBM that triples the qubit count when compared to its predecessor Eagle. According to IBM, this quantum chip can run any complex computational problem that a classical computer cannot. IBM is also working on to develop a 100,000 qubits quantum computer [4].
4. **AWS Ocelot**: Developed by Amazon that reduces the costs implementation of quantum error correction by 90% [5].

5. Quantum Algorithms

Quantum Algorithms are step by step process that enforce on quantum computers and uses principles of quantum mechanics like superposition, entanglement and interference that allows to us crack problems faster than classical algorithms. Quantum Algorithms can solve those problems in minutes which can take millions of years on fastest supercomputer. Some the well-known examples involve Shor Algorithm (for factorization) and Grover's algorithm (for search) demonstrated the power of quantum systems as compared to classical when solving some specific problems. Algorithms like VQE and QPE are used for healthcare that speeds up drug discovery process.
Some of the basic quantum algorithms discussed below:

- **Deutsch-Jozsa Algorithm:**

Proposed by David Deutsch and Richard Dozsa in 1994.This algorithm was the first prime example that shows quantum system outperforming classical system. It is concerned with specific type of problem but depicts the power of quantum parallelism.
For Example:
We are given a function(x) that takes an n-input and return either 0 or 1. Now we want to determine whether f is:
Constant → returns the same thing for all inputs, OR
Balanced → returns 0 for half the inputs and 1 for the different half.
Classically, in worst case we need to evaluate f(x) for 2^(n-1) + 1 inputs to be sure.
Deutsch-Jozsa Algorithm solves this using one evaluation of function by utilizing quantum system. It uses superposition for evaluating function on all inputs at the same time. Then using interference, it determines whether the function is constant or balanced.

This was the prime example of exponential speedup of a quantum algorithm and set the base for other future algorithms like Shor's Algorithm.

- **Shor's Algorithm:**

It was proposed by Peter Shor in 1994.It is concerned with solving integer factorization where a large integer is broken down into its prime factors. It was the first practical demonstration showing quantum system solving a problem exponentially faster than classical system.

For example:

Factorization of a 2048-bit number used in RSA encryption takes millions of years on fastest supercomputer since; classical systems hold exponential time to factor big numbers.

Shor's Algorithm completes it in polynomial time on a powerful quantum system. It sparked interest in post-quantum cryptography since it can break RSA encryption.

- **Grover's Algorithm:**

Luv Grover Developed Grover's Algorithm in 1996 which is designed for search optimization tasks. It shows quadratic speedup of quantum algorithms compared to classical.

For Example:

Let there be Unsorted Database D containing N items.

Let suppose we are trying to find specific item, then classical search would take N/2 item or linear time.

√N steps are required in Grover's Algorithm which is a quadratic speedup.

For example:

- Search by Classical Algorithms in 1,000,000 requires 500,000 checks.
- Grover's Algorithm requires 1,000 checks.

- **Berstein-Vazirani Algorithm:**

Ethan Bernstein and Umesh Vazirani proposed this algorithm in 1993 to show this as a proof-of-concept algorithm that demonstrates how quantum systems outperform classical systems (just like Deutsch-Jozsa).

For Example:

Let there be a function:

f(x)=a. x (mod 2)

where:

x: an n-bit input

a: hidden n-bit string

Problem: To find hidden string *a.*

On classical systems, function is queried n times which is once per bit of a, while on quantum system only one query is required to find *a*.

6. Quantum Computing and Healthcare

The field of Quantum Computing is set to revolutionize the Healthcare Industry. Quantum Computing can perform those tasks which are beyond the reach of a modern classical computer. Although, Quantum Technology has various use cases in the field of Healthcare, this paper mainly focuses on quantum drug discovery, its challenges, and future of quantum drug discovery.

Figure 4: A Typical Quantum Computer

Table 1 below depicts the differences between quantum and classical computing systems

Basis of Comparison	Classical Computing	Quantum Computing
Fundamental Unit of Storage	Bit (0 or 1)	Qubit (Superposition of 0 or 1).
Principle of Computation	Follows Boolean Logic i.e. Deterministic	Based on Principles of Quantum Mechanics i.e. Probabilistic.
Data Representation	Binary State (either 0 or 1) at a time.	Multiple states at the same time.
Processing	Either sequential or parallel (cores limitation).	Massive Parallelism through Quantum Entanglement.
Speed	Large and Complex Problems are slow on classical computers.	Exponential speedup for certain problems. Ideal for complex problems.
Stability	Mature Technology, hence low error rate.	In Developing stage, hence high rate of errors.
Applications	General Computing, databases, simulations.	AI, Drug development and other crucial areas like cryptography.

Table 1: Differences between Classical and Quantum Computing

7. Quantum Computing and Drug Discovery

Drug Discovery is a process of discovering new drugs or medicines. It involves several steps from detecting biological causes of a disease and developing compounds and verifying whether it is effective or not. History of drug discovery spans several millennia. Ancient Egyptian Papyrus provides around various methods to cure diseases.

Modern drug discovery has evolved substantially over recent decades. However, the process remains extremely costly and time-consuming—typically spanning 10 to 15 years and costing between $708 million (median) and $2.23 billion (average) to bring a new drug to market [6,7].

Development of a medicine takes place in several stages like relating a target, target validation, lead discovery, lead optimization, Pré-clinical and clinical testing, regulatory approval and post-marketing surveillance [8]. It takes around 10-15 years and billions of dollars to complete the development of drugs but, it leads to better health care system therefore, increasing life-expectancy of a nation.

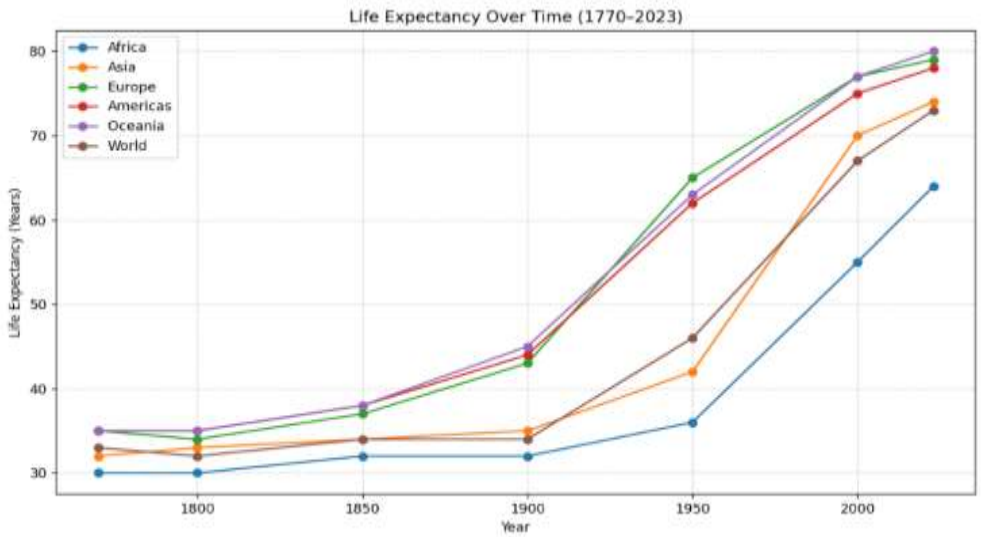

Figure 5: Global Life Expectancy Over the Time [9]

Figure 5 depicts the progress humanity has achieved in the field of medicine. The discovery of new drugs led to eradication of various diseases like polio and other thereby increasing global life expectancy. Although drug discovery led to curing of many diseases but the no. of processes involved in developing a drug is many and takes many years.

For example, it took around 35 years to develop a Malaria Cure which redounded in further losses in absence of any remedy [10].

Though Modern Drug is developed through MD and DFT by a method known as Computer Aided Drug Design (CADD), classical computers have limitations in simulating at the molecular level, since that would require many classical bits and would not be even completed in lifetime. Thus, Quantum Computers can accelerate the process because of superposition where a qubit can be in multiple states at a time, allowing faster and accurate computations leading to acceleration in evolution process.

Before moving to Quantum Computing Applications in Drug Discovery, we will first overview the steps in developing a drug.

A. DRUG DISCOVERY PROCESS

- **Target Identification:**
- This is the first step in drug discovery. A biological molecule such as a protein or a gene is identified which plays a key role in a disease.
- Targets are ought to be druggable i.e. which can be modulated by a small molecule or a biologic.
- Genomics, proteomics and disease association studies are used as sources.
- **Target Validation:**
- This step verifies that altering the target has desired therapeutic effect.
- Techniques include gene knockdown CRISPR editing and animal models.
- Goal is to demonstrate a causal relationship between target and disease.
- **Lead Discovery:**
- A library of compounds is screened using techniques like HTS or virtual screening to find hits that bind and effect
- These hits undergo biological assays to confirm activity and selectivity.

- Screening types include serendipitous discovery, random high-throughput discovery, molecular docking and virtual modeling and rational drug design.
- **Lead Optimization:**
- Chemists refine lead molecules to improve:
- Potency (lower dose needed).
- ADMET: Adsorption, Disruption, Metabolism, Excretion and Toxicity.
- This step may involve QSAR modeling or structure activity relationship studies.
- **Preclinical Development:**
  - Conducted in non-human such as cell structures and molecules.
  - Tasks Include:
    - Toxicity and Safety Profiling.
    - Pharmacokinetics (PK): How the drug moves through the body.
    - Formulation and close-range finding.
- **Clinical Trials:**
- Phase 0: Microdosing in humans to study PK IPD.
- Phase I: Safety and Tolerability in healthy volunteers (20-80 people).
- Phase II: Effectiveness and side-effects in patients (100-300 people).
- Post-approval surveillance to asses' long-term risks and rarer side.
- **Regulatory Review:**
- Full Data from pre-clinical phases are compiled into a New Drug (IND) submission.
- Regulatory bodies (like the FDA or CDSCO) review manufacturing efficacy, safety and labelling.
- **Post-Approval Monitoring:**
- Includes pharmacovigilance, real-world, evidence studies and possibly label expansions.
- Ensures ongoing compliance and detection of rare effects not seen trials.

Figure 6: Traditional Steps in Drug Discovery

B. CHALLENGES IN COMPUTER AIDED DRUG DISCOVERY (CADD)

Initially computers weren't utilized in medicine discovery. still, a conspicuous paradigm shift has passed with new languages like Computer backed Molecular Modeling (CAMM) and overarching concept called Computer Aided Drug Discovery (CADD) [11].

However, this technique has several limitations. CADD relies on traditional computing which struggles in bluffing complex molecular relations since classical bits can be either in any one state at a time. Quantum Computers can attack the problems that moment's computer struggle with [12].

The elaboration of Quantum Computing holds pledge for medicine discovery and development. Quantum generative models offer advantages by exhaustively covering distributions natural probabilistic nature [13].

Quantum Computers use laws of quantum mechanics, similar as superconducting circles (microwave oven radiation) or ions drifting within electromagnetic fields(lasers). QC uses quantum behavior to break the problems that cannot be really answered by classical computers [14].

Some of the challenges faced by CADD are:

- **Data Quality and Availability:** It is a critical challenge in drug discovery. Predictive Models depends on the datasets for accurate results which may be incomplete, contradictory leading to inaccurate predictions.
- **Complexity of Biological Systems:** Biological Systems are highly complex in nature. This makes analysis of interaction between drug candidate and body a significant challenge.
- **Computational Power and Efficiency**: Traditional Computers are incapable of simulating exponential complexity of molecules since traditional computers have limited computing power to simulate molecular interactions.
- **Interdisciplinary Collaboration:** CADD requires experts from various fields like biology, chemistry, computer science and pharmacology. Lack of interaction between the researchers can hinder the process thus, leading to delays and inefficiencies.
- **Predicting Drug Resistance and Efficacy:** One of the biggest challenges how the drug will perform in real world biological system.

C. QUANTUM SIMULATION

Quantum Simulation is a process of utilizing quantum systems to simulate the particles at molecular levels. Quantum simulation is a technique that possesses the ability to solve complex issues faced by traditional methods. It is a computational technique that uses various high-level, complex quantum algorithms to simulate and model complex molecule and material designs [15].

Simulating the quantum principles and phenomena accelerates the entire process of drug discovery since it allows to predict the behaviour of drugs, reduces the costs of producing a drug, better drug design and eliminating the need for hit and trial methods. Quantum Simulations mainly target large and complex molecules and are ideal for them but it also works in small molecules. Therefore, it can be applied on any type of drug.

D. MOLECULAR DOCKING

Molecule Docking is a computational methodology that is used to predict the binding or interaction between a small molecule(ligand) and the target(protein). This is used to identify an ideal drug candidate. Molecular docking in drug discovery synergistically employs sophisticated computational methodologies, encompassing CADD, QSAR, and advanced deep docking techniques [16].

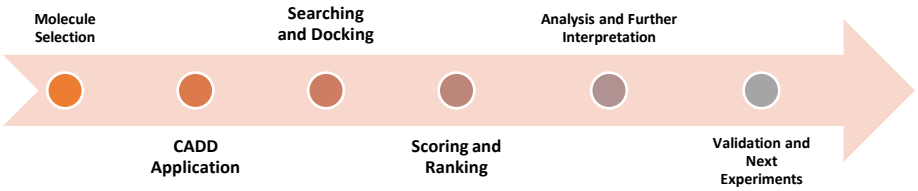

Figure 7: Molecular Docking Steps

The process of molecular docking is depicted in the figure 8 above
Molecular Docking consists of several steps

- **Molecule Selection**: Molecules are selected based on their potential drug-like attributed from various chemical databases.
- **CADD Application**: CADD is used to process the molecules to predict their pharmacological behaviour and optimization of interactions.
- **Searching and Docking**: Rotation and translations of ligands within the binding site to explore various confirmations and orientations.
- **Scoring and Ranking**: Best-fitting ligands are sorted and ranked based on their confirmation score of their binding energy for further analysis.
- **Analysis and Interpretation:** Top-ranked results are analysed to clear about the types of molecular interactions involved.
- **Validation and Next Experiments:** X-ray crystallography or list assays are used to validate ideal and suitable docking predictions.

Despite having colourful advantages molecular docking faces several critical challenges, and the integration of quantum computers holds pledge in addressing these issues [17].
Some of the challenges faced by classical molecular docking are given below:

- **Protein Flexibility:** Accuracy of binding predictions is limited since classical docking treats proteins and ligands as rigid structures despite they naturally modify their shape.
- **Simplified Solvation Methods:** Traditional Computing is slow and inefficient in simulating the effects of water and other solvents that are important in understanding the interaction between the molecules.
- **Computational Costs:** Molecular Docking of large biomolecules requires powerful systems therefore; the overall process is slow and resource-intensive.
- **Limited Accuracy in Binding Predictions:** Molecular interactions are used estimated using classical force fields which may be inaccurate especially in case of large or flexible molecules.
- **Restricted Exploration of Chemical Space:** Promising drug candidates may be ignored due to limited sampling of molecular configurations

Quantum computing can remove these drawbacks in the following ways:

1. **Modelling Protein Flexibility:** More realistic view of molecular interactions can be generated since quantum computers can simulate multiple protein confirmations.

2. **Advanced Solvation Simulation:** Solvent effects can be more accurately Modelled on quantum systems leading to Improved predictions of behaviour of drugs and binding stability.
3. **Quantum Mechanical Accuracy:** Quantum algorithms enhance prediction reliability by providing precise calculations of binding energies and molecular properties.
4. **Parallelism and Speed:** Quantum Computing processes docking simulations faster since it has ability to explore many possibilities at once
5. **Expanded Chemical Exploration:** Grover's algorithm a quantum algorithm can scan many chemical libraries that helps in uncovering novel drug candidates that might be overlooked by classical systems.

E. VIRTUAL SCREENING

Virtual Screening is a technique that is used for finding promising drug candidate by applying constraints on massive chemical libraries. This technique generally finds the potential candidate that can bind with specific biological target by performing analysis of molecular structure of several molecules. It is crucial in early-stage drug development process since, it filters many compounds, thus saving time and resources required because only those candidates are selected which show promising results.

Virtual Screening on classical systems have several limitations:

- Simplified models can be reason for incorrect predictions.
- Extensive Validation for Large False Positives.
- Difficult to explore large datasets due to high computational costs.
- Finding novel compounds is restricted to a large extent due to inadequate exploration of datasets/chemical space.

To develop potential drug compounds, we need to identify and understand the interaction of a target biomolecule, which can be achieved through virtual screening using QML [18].

QML is an interdisciplinary field that integrates and unites QC and machine learning to address complex problems [19].

Enhancements:

- **Quantum Simulations:** Quantum Systems can perform accurate modelling of molecular behaviour compared to classical systems. Accurate modelling is required in drug discovery since it allows researchers to study complex biochemical processes.
- **Quantum Feature Encoding:** The more compact the representation of molecules is, the more effective and briskly the analysis of implicit medicine campaigners. QML can render colourful molecular structures and properties in the quantum state [20].
- **Quantum Neural Networks:** Enhancing Prediction Accuracy by learning the complex patterns in the molecular data.
- **Quantum Kernels:** Quantum Kernels are used for improving classification tasks in protein(ligand)-based screening. This is done by capturing quantum correlations.
- **Quantum Search Algorithms:** Algorithms like Grover's Algorithm reduces screening time by searching through vast libraries.
- **Molecular Data Integration through Quantum:** For determination of molecular structures and properties of the complex, we use various processes and data technologies such as Nuclear Magnetic Resonance (NMR), X-ray and crystallography, and QML can be used to improve and increase its efficiency [21].

8. Challenges in Quantum Drug Discovery

Quantum Computing is a revolutionary technology that has potential to transform the landscape of pharmaceutical industry. We already have discussed above the performance of quantum computing and compared it against classical systems. Despite having great potential, discovery of drugs through quantum technology faces several challenges. Promising algorithms like VQE and QPE face several problems like scalability issues and optimization bottlenecks making them incompatible for modelling complex biomolecules (proteins or enzymes).

Another constraint is that quantum computing is still in nascent stage therefore, hardware configuration does not satisfy the requirements that would be required for drug discovery. Quantum Systems also suffer from stability issues. Therefore, today's quantum systems are only capable of simulating tiny molecules and not proteins (drug targets).

Some of the challenges faced by Quantum Systems in Drug Discovery:

A. HARDWARE LIMITATIONS:

- **Scalability:**

Quantum computers demand a great number of qubits to model complex molecular systems. The demand to have a system that needs a big number of coherent qubits poses a significant challenge regarding the scalability of the system [22].

For Example: IBM's Osprey quantum chip contains 433 qubits. For drug discovery, millions of error-corrected qubits are needed which still isn't achieved as of now. Organizations however, are rapidly working on developing better quantum chips with fault-tolerant qubits.

- **Error Mitigation:**

Error mitigation is another critical concern in quantum-assisted medicine discovery. Quantum computers are susceptible to inaccuracies due to decoherence and gate defects, impacting simulation precision [23].

- **Noise & Decoherence:**

Quantum bits lose their quantum state due to factors like environmental noise. We have discussed this property of quantum computing also known as decoherence which states the factors responsible for collapse in quantum state.

Decoherence is one of the biggest challenges in quantum technology since it may generate errors and difficult for performing large or complex calculations specially in case of drug discovery where small noise-induced deviations can generate inaccurate predictions

B. COST & ACCESSIBILITY:

Only major corporations like Google, IBM, Microsoft and others and well-funded pharma organizations have access to quantum technology because development and maintenance of quantum computers is costly. Thus, it restricts the global access of this technology which allows only few countries to access benefits of this technology.

C. ALGORITHMIC CONSTRAINTS:

Quantum Algorithms like Variational Quantum Eigen solver (VQE) and Quantum Phase Estimation works smoothly for simulation of small molecules but still has scalability issues i.e. in case of large and complex molecules resource needed grows exponentially thus, struggle to scale up better for real drug-sized molecules.

Problems of Both Algorithms discussed below:

- **VQE:** Suffers from Barren Plateaus also known as flat optimization landscapes where algorithm is unsuccessful in finding any accurate solutions because of systems getting larger and developing a flat region known as barren plateaus.
- **QPE:** It requires very deep circuits which is still not present on today's hardware. Also, current hardware is too noisy to handle it.

D. DATA QUALITY:

Huge datasets of chemical libraries, genomics and others are required in drug discovery. However, the data may be biased, incomplete or proprietary which reduces their value. Integration of quantum outputs with AI/ML pipelines is still Experimental.

E. REGULATORY COMPLIANCE:

Quantum-derived drug candidates lack standards for validating them. Pharmaceutical Industry is one of the most tightly regulated industry. There is need for standards and regulations before moving these drugs to real world clinical use.

F. INTERDICIPLINARY BARRIERS:

Drug Discovery and Quantum Computing in general are combination of various fields like Computer Science, Mathematics, Physics, Biology and Chemistry. Thus, it needs expertise from all domains.
Quantum Drug Discovery especially requires expertise from fields like biology, chemistry and computer science. Therefore, proper collaboration between researchers and experts from these fields are required since lack of it may hinder progress and researchers belonging to other domain main may not be able to analyse other's practical needs.

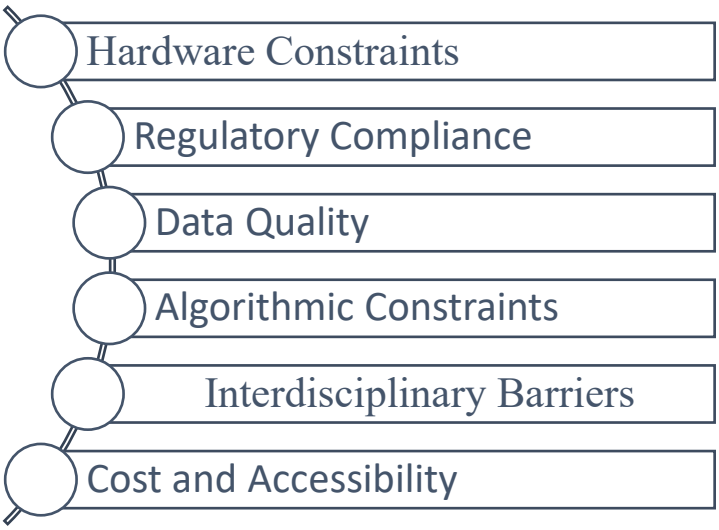

Figure 8: Challenges in Quantum Drug Discovery

9. Case Studies

Quantum Computing though, still in its early stage has great potential to change the course of drug development. Quantum Computer can perform more accurate simulations of molecular interactions. Here, we will discuss some case studies that depict the applications of quantum computing in drug discovery:

- **Quantum Embedded Graph Neural Network (GNN):**

Chinese Scientists made a breakthrough in August 2025 by developing a Quantum Embedded Graph Neural Network (GNN). It addresses the major constraints of prior models i.e. (they never concentrated on bond-level quantum interactions) by representing atoms as nodes and chemical bonds as edges at quantum level. The Researchers implemented this on Origin Wukong Quantum Computer. The system was able to maintain its stable performance on the noisy hardware currently used today and accuracy for predicting molecular properties improved which promises better efficiency in screening of drug candidate [24,25].

- **20x Speedup in Quantum Accelerated Drug Simulation:**

In June 2025 , IonQ partnered with AstraZeneca , AWS and Nvidia to demonstrate a quantum accelerated hybrid workflow that reduced simulation time by 20-folds for a reaction named Suzuki-Miyaura which is an important for small-molecule drug synthesis by integrating Forte quantum processor with Nvidia's Cuda-Q managed automatically via Amazon Braket and AWS Parallel Cluster, which enables the workflow to be completed within days instead of months while, maintaining accuracy .This depicted the efficiency and practicality of hybrid quantum-classical systems in early-stage drug development [26].

- **St. Jude and University of Toronto's Experiment on KRAS Protein:**

In April 2025, St. Jude's Children Hospital and University of Toronto collaborated to demonstrate a hybrid classical-quantum method to target KRAS protein, one of the most difficult to target often labelled as "undruggable". Aggressive cancers including pancreatic, lung and colorectal are due to KRAS mutations and always resisted traditional drug design strategies. The team of researchers developed a workflow that is capable of exploring large chemical spaces more efficiently than traditional methods by integration of quantum machine learning (QML) with classical models. This method produced several novel ligands, two of them experimentally confirmed to bind KRAS in laboratory experiments. This marks the first experimental validation of a quantum-assisted drug discovery [27].

- **IBM's Starling Project:**

IBM announced its project Starling in June 2025, which is designed to be fault-tolerant and scalable and can support up to 10,000 physical qubits by 2029. This system solves one of the major problems in current quantum hardware by incorporating a new error correction architecture that reduces logical errors when qubits are scaled up. Starling would be ideal for drug development, materials science and financial modelling since it is capable of performing 100 million accurate and reliable quantum operations [28].

- **Summary:**

Thus, the case studies demonstrate the current status and breakthroughs of quantum technology. China's Quantum GNN allows faster and accurate prediction of compound similarity while maintaining its stability. IonQ's hybrid quantum-classical workflow for simulating Suzuki-Miyaura reaction was reduced by 20 folds thereby, completing the entire workflow within days instead of months along with maintaining its accuracy. In the same way, quantum models were applied to target KRAS protein in a method by St. Jude's Children's Research Hospital which identified several binding ligands, where two of them were experimentally validated. It is also worth to mention IBM's Starling project which aims to develop a fault tolerant and scalable qubit system by incorporating a new error correction architecture.

10. Future Scope

Quantum Technology in future can become finally mainstream in developing drugs since it accelerates the process by allowing accurate predictions and simulation of complex biomolecules. These systems can

execute them in few minutes to hours compared to classical systems. Here are some of the advancements that are expected in future:

1. Evolution of Quantum Hardware:

Today's Quantum Hardware is still incapable for simulating complex biomolecules because of insufficient qubits. Also, Current Systems belong to Noisy Intermediate Quantum Scale Era which means qubits aren't error corrected. Future Systems must focus on scaling up qubits and developing error corrected qubits. With more error corrected qubits quantum systems will become capable of performing complex and large-scale simulations. A quantum system with millions of qubits is expected in future that will easily be capable of performing complex simulations.

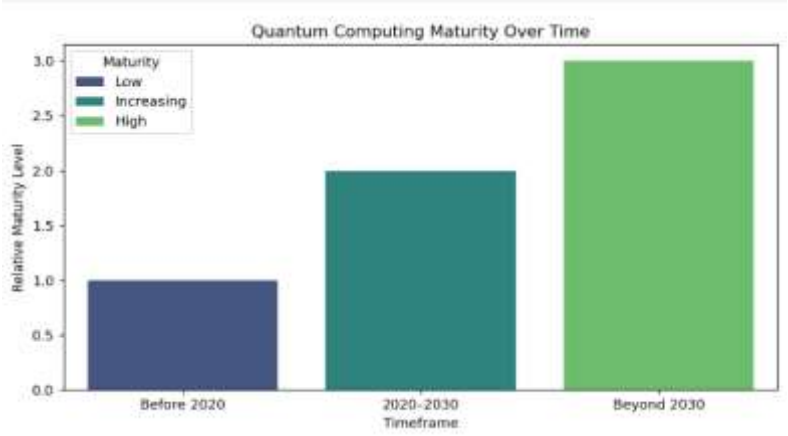

Figure 9: Evolution and Future of Quantum Technology [29]

Table 2 : Table Elaborating the Growth of Quantum Technology as depicted in Figure [Source: McKinsey].

Phase	Time	Maturity	Key Activities	Funded By
Inception	Before 2020	Low	Fundamental Research and Development of Technology Academic and Early commercial activities Emergence of quantum-inspired Algorithms. Disruptive Changes.	Government or Pioneer Investors.
Not Fully Error Corrected QC	From 2020-2030	Increase-sing	Early Commercialization and Commercial R & D Business Development Incremental and Disruptive Changes	Corporate R & D. Venture Capital Governments
Fully Error Corrected QC	Beyond 2030	High	Full Value Creation Commercial Rollout	Value-Based Pricing

			Dominance of Incremental innovations.	

2. Industry Regulations:

Currently, there exists no regulations for quantum-derived drug candidates. Pharma Industry is highly regulated and seen by agencies like U.S. Food and Drug Administration (FDA) and European Medicines Agency (EMA). Even though how accurate the quantum results may be, they still have to be verified through classical simulations, preclinical studies and clinical trials. Therefore, a proper clinical framework is required for utilizing quantum system into pharmaceutical industry since, without any regulations quantum derived drugs may face delays in getting approval for use.

3. Hybrid Quantum Systems:

Integration of Quantum Computing with high-performance classical computers and artificial intelligence is crucial for accelerating drug discovery process. Quantum systems are expected to work as hybrid systems in future. Hybrid Systems would divide complex tasks into specialized sub-tasks i.e. preprocessing of data at large scale would be handled by classical computer, artificial intelligence can be utilized in decision-making and optimized learning and quantum systems would perform simulations of molecular interactions. This has potential to bring revolution in personalized medicine, since drug efficacy and toxicity can be determined at individual's genome level and clinical history.

We already gave an example of Utilization of Hybrid Quantum Systems in our case study section.

11. Conclusion

This paper depicted the advantages of Quantum Technology over Traditional especially in case of drug discovery. Quantum Systems are soon to make many breakthroughs in the field of drug discovery and other crucial areas like cryptography. In case of drug discovery Quantum Technology would bring revolution by integrating AI-driven Drug Design, allowing accurate molecular simulations and quick reaction modelling.

Although, there exists some challenges like hardware limitations, noise and decoherence, maintenance there are still breakthroughs in quantum drug discovery as shown by above case studies. Therefore, these challenges must be addressed before making quantum computing mainstream for developing drugs in pharmaceutical industry.

12. Glossary of Selected Terms

1. Molecular Dynamic Simulations (MDS):

A computational technique that helps to model the behaviour of biological molecules such as proteins, enzymes and drug compounds over time by applying Newton's law of motion on atoms and molecules to simulate their movement and response to external factors like forces, temperature and pressure.

MDS assists scientists in examining the binding behaviour between the drug and its target protein, structural stability prediction and identification of energetically favourable conformations.

2. Quantum Annealing:

A special type of quantum computation concerned with solving optimization statements by searching lowest-energy configuration of system. It utilizes superposition and tunnelling for determining various configurations simultaneously. Algorithm anneals into optimal state and finds best solutions out of many

possibilities. Quantum annealers optimizes molecular docking, reaction pathways and compound screening where exists multiple energy minima.

3. Quantum Integrated Clinical Trials:

An emerging Interdisciplinary framework that integrates quantum computing, artificial intelligence and clinical data science for revolutionizing the design and execution of pharmaceutical trials. Incorporates quantum-enhanced simulations to predict patent-specific responses and trial parameters to boost up drug development process. Personalized medicines can also be developed through this approach by combining molecular-level modelling with real world clinical data which results in improved accuracy and efficiency.

13. References

1. IBM. (2025). *What is quantum computing? * IBM Think. Retrieved from https://www.ibm.com/think/topics/quantum-computing
2. Microsoft. (2025, January 17). *Introducing Majorana-1: Microsoft's first topological quantum chip. * Microsoft Official Blog. Retrieved from https://blogs.microsoft.com/blog/2025/01/17/majorana-1-quantum-chip
3. Google Quantum AI. (2025, June). *Google's Willow: A new quantum processor that outperforms supercomputers. * Google Research Blog. Retrieved from https://blog.research.google/2025/06/google-willow-quantum-chip
4. IBM Research. (2022, November 9). *IBM Osprey: Our 433-qubit processor. * IBM Research Blog. Retrieved from https://research.ibm.com/blog/433-qubit-processor-ibm-quantum
5. Amazon Web Services. (2025, February 27). *Amazon Web Services announces a new quantum computing chip. * AWS News.
6. PhRMA & BIO. (2022). *What is the average time to bring a drug to market in 2022? * N-SIDE Life Sciences Blog. Retrieved from https://lifesciences.n-side.com/blog/what-is-the-average-time-to-bring-a-drug-to-market-in-2022
7. Deloitte. (2025, March 25). *Drug development cost pharma $2.2B per asset in 2024 as GLP-1s drive financial return. * Fierce Biotech. Retrieved from https://www.fiercebiotech.com/biotech/drug-development-cost-pharma-22b-asset-2024-plus-how-glp-1s-impact-roi-deloitte
8. Martínez, M. (2025, March 26). *Drug discovery and development: A step-by-step process. * ZeClinics Blog.
9. Dattani, S., Rodés-Guirao, L., Ritchie, H., Ortiz-Ospina, E., & Roser, M. (2023). *Life expectancy. * Our World in Data. Retrieved from https://ourworldindata.org/life-expectancy
10. Smithsonian Magazine. (2022, June). *Why did it take 35 years to get a malaria vaccine? * Smithsonian Magazine. Retrieved from https://www.smithsonianmag.com/science-nature/why-did-it-take-35-years-to-get-a-malaria-vaccine-180980151/
11. Crumblearn. (2025, February 25). *Introduction – Computer aided drug discovery (CADD). * Retrieved from https://cadd.crumblearn.org/intro/
12. Rajendran, V. D., Swaminathan, B., Washington, S. G., Dhandapani, A., & Jeevanesan, V. (2024, July). Applications of quantum computing in drug design and molecular simulation. *YMER, 23*(7), 31–38. Retrieved from https://ymerdigital.com/uploads/YMER240731.pdf
13. Biswas, R., Basu, A., Nandy, A., Deb, A., Haque, K., & Chanda, D. (2020, February). Drug discovery and drug identification using AI. In *Proceedings of Indo–Taiwan 2nd International Conference on Computing, Analytics and Networking (ICAN)* (pp. 49–51).

14. Srivastava, R. (2023, December). Quantum computing in drug discovery. *Information System and Smart City, 3*(1). https://doi.org/10.59400/issc.v3i1.294
15. Ma, H., Govoni, M., & Galli, G. (2020, July). Quantum simulations of materials on near-term quantum computers. *NPJ Computational Materials, 6*(1), 1–8.
16. Gentile, F., Yaacoub, J. C., Gleave, J., Fernandez, M., Ton, A.-T., Ban, F., Stern, A., & Cherkasov, A. (2022, March). Artificial intelligence–enabled virtual screening of ultra-large chemical libraries with deep docking. *Nature Protocols, 17*(3), 672–697.
17. Bernal, D. E., Ajagekar, A., Harwood, S. M., Stober, S. T., Trenev, D., & You, F. (2022, June). Perspectives of quantum computing for chemical engineering. *AIChE Journal, 68*(6), e17651.
18. Mensa, S., Sahin, E., Tacchino, F., Barkoutsos, P. K., & Tavernelli, I. (2023, March). Quantum machine learning framework for virtual screening in drug discovery: A prospective quantum advantage. *Machine Learning: Science and Technology, 4*(1), 015023.
19. Gorgulla, C., Jayaraj, A., Fackeldey, K., & Arthanari, H. (2022, August). Emerging frontiers in virtual drug discovery: From quantum mechanical methods to deep learning approaches. *Current Opinion in Chemical Biology, 69*, 102156.
20. Yano, H., Suzuki, Y., Itoh, K. M., Raymond, R., & Yamamoto, N. (2021). Efficient discrete feature encoding for variational quantum classifier. *IEEE Transactions on Quantum Engineering, 2*, 1–14.
21. Kumar, G., Guizani, M., Yadav, S., Mukherjee, A., & Hassija, V. (2024, March). Recent advances in quantum computing for drug discovery and development. *IEEE Access, 12*, 64491–64503. https://doi.org/10.1109/ACCESS.2024.3376408
22. Lolur, P., Skogh, M., Dobrautz, W., Warren, C., Biznárová, J., Osman, A., Tancredi, G., Wendin, G., Bylander, J., & Rahm, M. (2023, February). Reference-state error mitigation: A strategy for high accuracy quantum computation of chemistry. *Journal of Chemical Theory and Computation, 19*(3), 783–789.
23. Endo, S., Cai, Z., Benjamin, S. C., & Yuan, X. (2021, March). Hybrid quantum-classical algorithms and quantum error mitigation. *Journal of the Physical Society of Japan, 90*(3), 032001.
24. CGTN. (2025, August 12). *China makes breakthrough in quantum computing for drug discovery. * Retrieved from https://news.cgtn.com/news/2025-08-12/China-makes-breakthrough-in-quantum-computing-for-drug-discovery-1FM3q3NLCPm/p.html
25. Digital Watch Observatory. (2025, August 14). *China debuts quantum-embedded GNN for drug discovery. * Digital Watch Updates. Retrieved from https://dig.watch/updates/china-debuts-quantum-embedded-gnn-for-drug-discovery
26. The Quantum Insider. (2025, June 9). *IonQ speeds quantum-accelerated drug development application in partnership with AstraZeneca, AWS and NVIDIA. * Retrieved from https://thequantuminsider.com/2025/06/09/ionq-speeds-quantum-accelerated-drug-development-application-in-partnership-with-astrazeneca-aws-and-nvidia/
27. Generous, A. (2025, April 3). *Quantum computing makes waves in drug discovery. * St. Jude Children's Research Hospital. Retrieved from https://www.stjude.org/research/progress/2025/quantum-computing-makes-waves-in-drug-discovery.html
28. Coxworth, B. (2025, June 10). *IBM will build 'monster' 10,000-qubit quantum computer by 2029 after solving science behind fault tolerance. * Live Science. Retrieved from https://www.livescience.com/technology/computing/ibm-will-build-monster-10

29. M. Evers, A. Heid, and I. Ostojic, "Pharma's digital Rx: Quantum computing in drug research and development," *McKinsey & Company*, Jun. 18, 2021. [Online]. Available: https://www.mckinsey.com/capabilities/life-sciences/our-insights/pharmas-digital-rx-quantum-computing-in-drug-research-and-development