How Quantum Computing System Size and Performance Enhances the Drug Discovery Process for KRAS Mutants

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Abstract:
This study discusses the role of quantum computing in the drug discovery process for KRAS mutants and how larger qubit counts and increases in circuit depth can enhance the process. Increasing system size may offer improvements in the coming years. Specifically, as quantum computing enters the fault-tolerant era, algorithms requiring error-correction due to their long runtimes and sensitivity to noise can be used. By increasing the number of high-fidelity operations compared to today's error-prone quantum computers, fault-tolerant systems will enable new classes of more capable algorithms and enhanced discovery of KRAS inhibitors. Lowering maintenance costs and increasing accessibility of quantum computers are necessary for a larger population to be able to make more rapid advancements in the field.

Introduction:

From the Altair 8800 in 1975 to the powerful multi-use machines available today, computers have had an undeniable impact on human life. Classical computer systems are computers that operate through the use of binary 0 and 1 code, and make up virtually all of the computers that the world uses today. However, a novel computing system is under rapid development: quantum computing. Unlike classical computers that operate using bits that have a binary value (i.e. 0 or 1), quantum computers operate using qubits, which harness the quantum mechanical properties of superposition and entanglement to exist in a simultaneous state of being both 0 and 1. When measured, a qubit collapses into one definitive value, which is dependent on the probabilities of each value.

The quantum mechanics of superposition and measurement determine the probability that a qubit will be 0 or 1 when measured. Quantum entanglement is another phenomenon that contributes to the immense computational power of quantum systems. Entanglement is a type of correlation that allows for an operation on one qubit to instantly affect other entangled qubits despite being vast distances apart [28]. The main factor of this computational power and the computational advantage over classical computers is a property called magic. Magic is the property of entangled qubits that makes their state unable to be effectively simulated on a classical computer [22]. The amount of "magic" in a system is determined by how many non-Clifford gates, quantum gates that cannot be simulated efficiently on a classical computer, are needed to represent it. Non-Clifford gates can be simulated with classical systems, but magic leads to exponential resource requirements to represent quantum states which limits the amount of non-Clifford gates able to be simulated on a classical computer. For example, if a quantum computer were able to represent quantum states with N qubits, a classical computer

would require 2N complex numbers to represent that same state. It is these gates that give quantum computers the computational edge over their classical counterparts.

A qubit can be thought of as any physical system that behaves like a two-state quantum system (ground and excited states that can exist in superposition) [2]. While there are many types of qubits, three of the most studied qubit types are spin qubits, superconducting qubits, and photonic qubits. [1]. Spin qubits use the spin (a quantum property that represents angular momentum) of an atomic nucleus or an electron as a qubit. Spin qubits are known for their robustness due to the relative stability of the quantum state of a spin against external interference [27]. Electron spin qubits are more suitable for being used in quantum processors since they can be manipulated and coupled to other electrons much quicker than nuclear spin qubits, and nuclear spin qubits are more suitable for quantum memory applications due to their much longer coherence time—the duration over which a qubit maintains its quantum information before external influences cause information loss—compared to electron spin qubits [27]. The interaction between an electron spin and a nuclear spin in order to transfer quantum information between the two is called hyperfine coupling, an interaction that is necessary for spin qubit application in quantum information processing [27]. Superconducting qubits are built from superconducting materials, which provide zero electrical resistance when cooled to an extremely low temperature. Photonic qubits may be prepared in multiple ways. They can utilize the polarization state of a photon—the orientation of a photon's electrical field as it travels—to represent a qubit state. They can also use a bosonic approach, where logical qubits are encoded into a single bosonic mode of the electromagnetic field. The quantum state of that bosonic mode is being manipulated by optical elements, and each mode can hold any number of photons. Both of these approaches represent different encoding methods in photonic quantum computing.

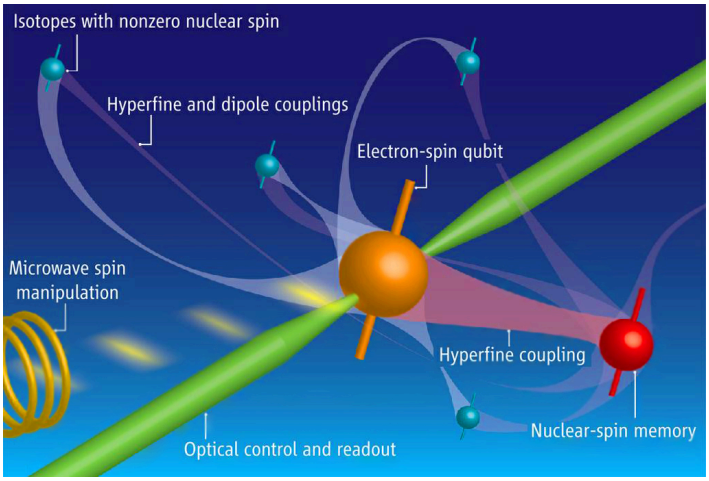


Diagram of an electron spin qubit coupled to a nearby nuclear spin through hyperfine coupling. This coupling enables quantum processing and storage within the system.

Photo credit: Christoph Boehme, Dane R. McCamey, Science Magazine

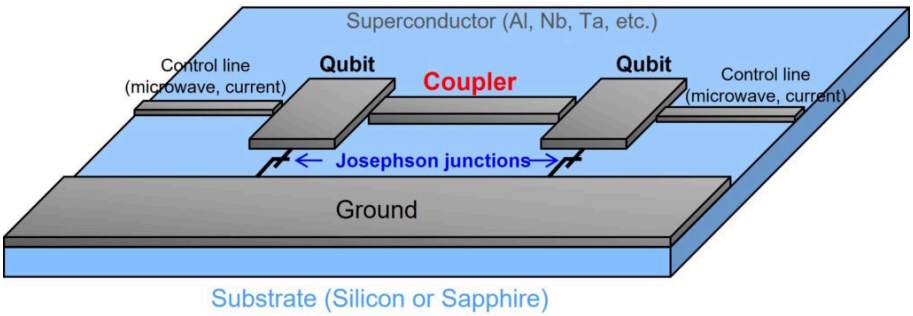


Diagram of a superconducting quantum processor. Each qubit is formed from superconducting material and coupled through Josephson junctions (quantum devices made of two superconductors that are separated by a thin insulating barrier). Microwave control lines are used for qubit manipulation and readout.
Photo credit: Toshiba Corporation

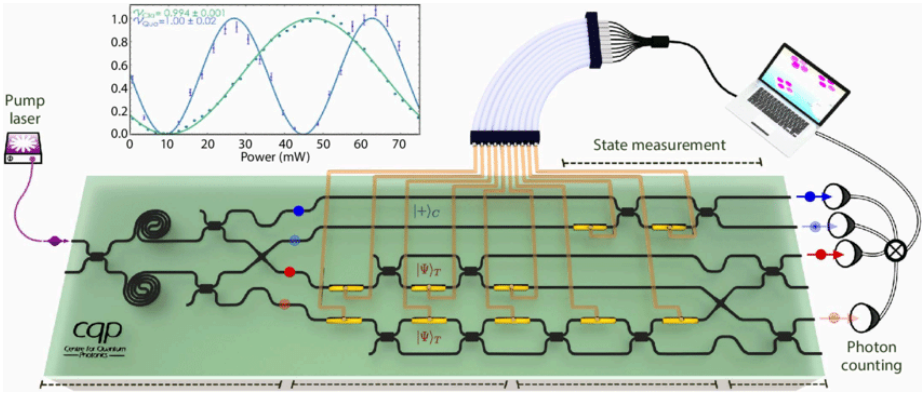


Diagram of a silicon quantum photonic processor where qubits are encoded in photonic states and manipulated with optical components. Measurement is performed through photon counting at the output.
Photo credit: Raffaele Santagati, Jianwei Wang, Antonio Andrea Gentile, Stefano Paesani, ResearchGate

In order for a quantum computer to be able to function properly, unwanted interactions with the environment, or noise, must be minimized in order to maintain each qubits' superpositional state. Some examples of external interference include electromagnetic signals and cosmic rays. These effects can lead to the derangement of a qubit's quantum state, a process known as decoherence. Shielding qubits from their environment requires extremely precise control mechanisms and regulated temperatures, which are very difficult and expensive to implement and maintain for systems with many qubits. In essence, bigger quantum systems require increasingly more effort, money, and precision to be able to keep qubits in a coherent quantum state, which in turn limits the maximum system size a quantum system can be.

Noisy Intermediate Scale Quantum (NISQ) devices consist of anywhere between 50 to 1,000 qubits. As system sizes scale and we enter the early fault-tolerant era, a distinction must be made between two different types of qubits: physical and logical. Physical qubits are the actual error-prone hardware, such as the qubits mentioned earlier, whereas a logical qubit is an entangled group of physical qubits that is made more stable and resistant to errors through the use of an error-correcting code [25]. As the frontier for the total possible number of qubits to be used and operations able to be run grows, and as deeper quantum circuits become more accessible, it becomes increasingly important to prevent decoherence. Today, the error rates for modern quantum computers typically lie between 1% and 0.1%. However, as error correction models increase in prominence, this percentage is expected to shrink to ever-so-small proportions: the error rate for algorithms with known quantum advantage must lie between 10-2 and 10-6, depending on the noise model [29]. In July 2025, scientists hit a quantum error rate of 1.510-5, an unprecedentedly low rate [3].

A quantum-classical model utilizes the strengths of both quantum and classical computing to achieve tasks typically more complex than what can be done with a pure classical or quantum machine. This is because of the problems of quantum noise and decoherence that become increasingly detrimental as the size of the quantum system grows. Quantum-classical systems are typically more optimal today, as they interface classical elements to reduce the depth of the quantum circuit and thereby limit the effect of noise on the computation. These systems are stopgap solutions that allow us to seek quantum advantage with current NISQ hardware.

Today, quantum computing is used in an increasing number of professions and tasks, such as finance tracking and management, materials science, integration with AI to create hybrid models, and many others. Currently, major companies such as Google, Microsoft, IBM, and Amazon utilize quantum computing to enhance their operations. Based on their roadmaps and timelines, these companies expect quantum technologies to improve in their respective tasks through reduced error rates, larger system sizes, and the development of hybrid quantum and classical models [5].

The pharmaceutical and biotech industries have also adopted quantum computing for tasks including materials science, genomics, catalyst modeling, and drug discovery. The intersection between the field of drug discovery and quantum computing occurred quite recently, with the first quantum computing algorithm designed for drug discovery being developed in 2001 [26]. Since then, many new innovations and quantum computing algorithms have allowed for potential quantum advantage, which describes when a quantum computer is able to outperform a classical computer at a specific task, to occur in areas such as medical imaging, data security, personalized medicine, and drug discovery; the rest of this paper focuses solely on quantum computing’s implications in drug discovery.

Research Question:
Quantum computing has the potential to offer significant benefits to the efficiency and effectiveness of drug discovery. In principle, quantum computers have the capability to explore massive numbers of molecular structures through specialized algorithms, significantly decreasing time and energy spent. One process in which quantum approaches have been explored is the generative modeling of molecules. Because quantum computers are able to more efficiently emulate quantum systems compared to classical computers, quantum algorithms are better able to model molecular interactions between drugs and targets with a greater degree of precision [6]. This enhanced generative modeling coupled with more realistic simulations can help in developing new drugs for constantly mutating targets [7].

Beyond molecular modeling, quantum computing is able to improve protein folding predictions, speed up search for molecules with high binding affinities with the target, aid in large-scale data management and analysis, and optimize development of personalized medicines [6]. Furthermore, the cost savings that quantum computing offers are substantial. As of early 2024, biopharma companies spent over $2 billion on average to discover, develop, and commercialize a new drug [7]. Roughly 30% of this total cost can be saved when utilizing quantum computing [8], and quantum computing interfaced with drug discovery is projected to have an overall economic impact of $700 billion by 2035 [7].

What is KRAS?
KRAS, short for Kirsten rat sarcoma viral oncogene homolog, is a gene that makes a protein that is responsible for regulating the growth, development, and death of cells in the body. The natural, unchanged form of this gene is known as the wild-type for KRAS. However, KRAS is also a frequently mutated oncogene, present in a variety of cancers including lung, colorectal, and pancreatic cancer [9]. KRAS has been difficult to target therapeutically, due to its complex nature and lack of deep binding pockets for a drug. Consequently, KRAS inhibitor research has become a promising avenue of future development for computational methods including classical, hybrid quantum-classical, and future-term quantum algorithms.

Quantum Algorithms
A variety of quantum algorithms can be applied to the KRAS inhibitor discovery process. Quantum annealing is a heuristic algorithm that is used to find the lowest-energy binding configuration in a system [21]. It can be used in KRAS inhibitor discovery to identify optimal ligand conformations that minimize the interaction energy between a candidate molecule and the KRAS protein. The Variational Quantum Eigensolver (VQE) algorithm is used to determine the ground states of molecules, information essential for accurate chemical simulations, which enables more accurate predictions of binding energies for drug-like molecules. Quantum Circuit Born Machines (QCBM) are algorithms that learn unknown probability distributions of a given

dataset to then generate new samples in accordance with that data [24]. It is essential to note that although QCBMs generate new samples, they do not explicitly compute system properties or physical observables, they merely learn and generate from existing probabilities. Consequently, in KRAS inhibitor discovery applications, QCBMs are primarily used in the early-stage candidate generation phase, as is seen in the following section. There also exists an algorithm known as QPE (Quantum Phase Estimation), which similar to VQE is also used to calculate the ground-state energy of molecules. We will discuss QPE in greater detail further into the paper.

Algorithm	**Function (general)**	**Function (KRAS-specific)**
Quantum Annealing	Identifying lowest-energy binding configuration	Minimizing interaction energy between candidate and KRAS protein
Variational Quantum Eigensolver (VQE)	Determining the ground states of molecules	Precise binding energy predictions for drug-like molecules
Quantum Circuit Born Machines (QCBM)	Generating new samples from learning the unknown probability distribution of a given dataset	Early-stage candidate generation phase
Quantum Phase Estimation	Like VQE, also calculates ground-state energies	Detailed further into the paper

The table outlines various quantum algorithms, their general functions, and their specific applications in KRAS inhibitor discovery

If you were to scale the qubit count for these algorithms used in KRAS inhibitor research, what would improve? Can the process be made more efficient with current hardware? Are there consequences for introducing such algorithms? The rest of this paper will answer these questions by examining a recent breakthrough in the field of KRAS inhibitor discovery through the integration of quantum computing, then looking at the consequences and limitations of this integration.

Methodology and Study:
As of November 2025, there are two FDA-approved KRAS inhibitors available for clinical use: sotorasib and adagrasib. They began to be developed both in 2013 after a discovery of a druggable pocket on the G12C mutant of KRAS [23]. Sotorasib was approved by the FDA in May 2021 and adagrasib in December 2022. However, in December 2024, a hybrid quantum-classical algorithm discovered two potential KRAS inhibitors that met the criteria for further development and possible clinical use in the future [9].

The process for discovering these candidates involved three main stages. First, a dataset of around 650 previously known KRAS inhibitors was created, where then classical and quantum-classical algorithms added roughly a million more structurally-similar molecules. With over 1 million possible drug candidates, the dataset was used to train the quantum-classical generative model that ultimately designed the KRAS inhibitors. The second stage of the process used the generative model, a combination of a QCBM with a 16-qubit processor and a classical long short-term memory (LSTM) network to generate around 1 million new molecules. In the third stage, these 1 million new compounds were first sampled and screened for pharmacological viability and ranked based on their protein-ligand interaction (PLI) scores, where a higher score meant a stronger binding affinity. Then, the 15 candidates with the highest PLI scores were synthesized and tested via experimental methods that provide insight into how a molecule will perform in a more complex biological environment. Of these 15 candidates, two molecules demonstrated significant promise as KRAS inhibitors: ISM061-018-2 and ISM061-022.

The application of quantum computing elements in the KRAS ligand development process resulted in significant time, energy, and money savings. The hybrid generative model was able to more effectively generate high-quality samples. In fact, the molecules generated by the QCBM-LSTM model resulted in around a 21.5% improvement in passing filters that assessed stability and synthesizability compared to if a purely classical LSTM model had been used [9]. This efficiency resulted in a shorter period of preclinical discovery, significantly lowering costs, energy, and time.

However, the discovery process for these two candidates would not have been significantly improved by running the QCBM on a processor with more than 16 qubits. This is because of an inherent limitation of QCBMs. QCBMs are a specific type of algorithm known as variational algorithms. In essence, these variational algorithms consist of a series of parameterized quantum circuits that are all trying to guess the correct quantum state needed in solving a problem. Each of these guesses are then refined by classical methods to find an approximate solution. As the system size of a variational algorithm increases, there needs to be more parameters. More parameters signifies a higher dimensional space being explored, and variational algorithms become less useful when the dimensions of the search space are high.

Optimizing the parameters of quantum circuits requires significant time, so including more parameters makes it harder for VQAs to find optimal solutions. The issue of barren plateaus (regions in the variational optimization landscape where gradients become very small) also arises, resulting in the algorithm getting stuck in regions of bad solutions or no solutions. Moreover, VQAs are not the most robust when it comes to noise mitigation, especially as complexity increases, which also acts as a significant limiting factor for QCBMs [14]. Current research indicates that these limitations are significant enough to require novel approaches.

Quantum computing itself needs to enter a new era, an era known as the MegaQuop Era (early fault-tolerant quantum computing). Expected to consist of tens of thousands to over a million physical qubits, MegaQuop quantum computers involve quantum processors executing up to a million quantum operations before error affects computation [15]. Though considerable progress for achieving this stage in quantum computing has been made, MegaQuop computers do not exist today and remain as a goal for the near future. They offer significant advantages compared to NISQ computers, such as the ability to explore significantly higher dimensional spaces than what QCBMs can efficiently explore by incorporating significant quantum error correction. This heightened exploration can speed up the steps of drug discovery, from faster simulations to better drug binding predictions. MegaQuop will be the next big step towards more efficient KRAS inhibitor research, and will bring us closer to achieving the ideal fully fault tolerant quantum computer.

When this new era of quantum computing is achieved, there will be novel FTQC (fault-tolerant quantum computing) approaches that could possibly replace or outperform QCBMs in the process of discovering KRAS inhibitors. The main issue with the current QCBM and generative machine learning hybrid model is that it is a mere heuristic, using probability distributions to generate data, not physical observables such as molecular ground-state energies [16]. Thus, a more precise fault-tolerant approach that could replace QCBMs is QPE (Quantum Phase Estimation). QPE can compute the eigenvalues of molecules with a guaranteed level of accuracy [17]. Accurately knowing the ground-state energies, reaction profiles, and potential energy surfaces of a molecule offers a key advantage over QCBMs in reliably predicting a drug's binding affinity and interactions with its target, making it a promising future replacement for QCBMs in the new molecule generation phase of KRAS inhibitor research. However, QPE is heavily resource intensive, requiring deep circuits and many logical qubits [18].

A less intensive approach that uses shallower circuits yet is still systematically improvable are Quantum Krylov Subspace and Diagonalization methods. These algorithms work by first preparing an initial quantum state and then allowing it to evolve under the system's energy structure for several short time intervals to record how the state changes [19]. The algorithm will then collect a small set of the states that captured the most important energy behavior, resulting in a low-dimensional space known as the Krylov subspace [19]. Finally, the algorithm will

calculate how strongly these states are related to one another and feed the info to a classical computer, which will extract the approximate energy levels [19]. This Krylov subspace approach is also more realistic for the near future, as it is more feasible for near-term or MegaQuOp hardware as opposed to needing full fault tolerance to operate efficiently.

Another MegaQuOp approach is a variant of VQE that uses only some fault tolerance to give better and more reliable results than NISQ VQE. These variants, like the Krylov Subspace and Diagonalization methods, also can replace QCBMs for tasks that require physics-based energy calculations. However, they cannot replace them for generative and explorative tasks. It is also important to note that in order for fully fault-tolerant machines to have realistic Hamiltonian (time evolution) simulations, techniques such as qubitization and advanced factoring must be implemented [20]. These techniques result in higher precision with fewer machine resources, breaking down chemical Hamiltonians into smaller pieces and compressing symmetrical molecular interactions [20]. Without these techniques, realistic chemical simulations will be too slow and expensive even for fault-tolerant quantum computers to simulate.

Approach to replace QCBMs	**Function**	**Feasibility in near-future use**
Quantum Phase Estimation (QPE)	Can accurately compute the ground-state energies, reaction profiles, and potential energy surfaces of a molecule	Not feasible for near-future or MegaQuOp: heavily resource intensive, requires deep circuits and many logical qubits
Quantum Krylov Subspace and Diagonalization Methods	Extracts the approximate energy levels with the help of a classical computer	Feasible for near-term or MegaQuOp hardware, does not require full fault-tolerance
MegaQuOp VQE Variants	VQE variants developed for MegaQuOp machines, improvement in precision and circuit depth from NISQ VQE	Feasible for near-term or MegaQuOp hardware, does not require full fault-tolerance

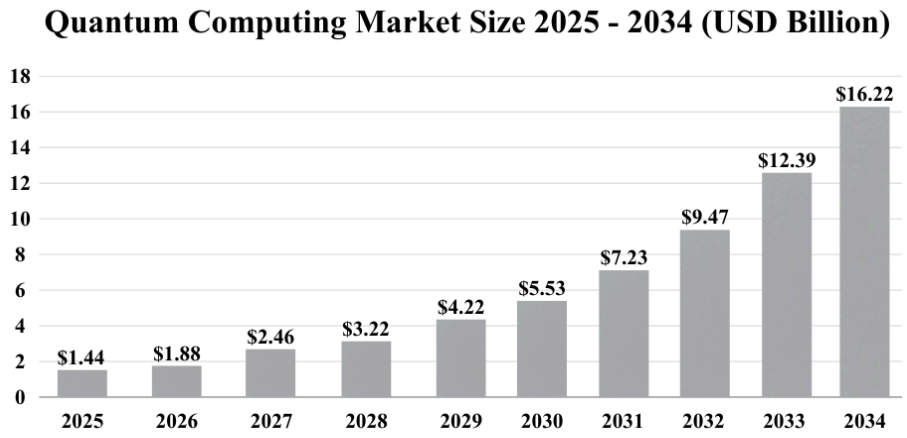
The table outlines various alternative quantum algorithms that could replace QCBMs in the KRAS inhibitor discovery process in the future. It outlines feasibility for near-term use and the varying levels of precision for the different algorithms.

Evaluation of Study:

Despite the promise quantum computing brings to the field of KRAS inhibitor and drug discovery as a whole, several limitations arise with the large-scale adoption of quantum technology into the industry. Despite the improvements quantum technology brings to the field, drug discovery

still requires a significant amount of money, which isn't attainable for smaller institutions and research facilities. This results in economic inequality and a widening gap between nations and institutions that have and do not have access to quantum technology, and the latter will have less access to novel pharmaceutical remedies and therapies acquired through the integration of quantum systems. This does not apply solely to biopharma companies with drug discovery, but with any company looking to integrate quantum tech into their pipelines. The estimated cost for just a singular superconducting qubit is between $10,000 to $50,000, while a fully operational quantum computer can cost tens of millions of dollars [12], meaning that quantum technology is simply not accessible for many institutions, facilities, and nations.

There also exists a shortage of qualified individuals qualified to work with quantum computers due to the highly specialized knowledge required for it [11]. In a recent study conducted by BBC Research, the quantum computing market is expected to grow from $1.6 billion in 2025 to $7.3 billion by 2030, with an associated compound annual growth rate of 34.6% [4]. Yet at the same time, deployment costs are only increasing. If not solved soon, the problem of shortage of talent may become the primary obstruction of quantum computing research.



Projected growth of the global quantum computing market from 2025 to 2034, indicating rapid industry expansion.

Data adapted from Precedence Research

Implications for future research:
Firstly, further investigation into the two candidates found in the December 2024 study must be conducted to acquire information regarding their mechanisms of action, and cocrystallization studies must be conducted to validate these mechanisms. There also exists quantum simulations that can be used to accurately predict its mechanisms of action, where computational results match closely with laboratory findings. In terms of quantum computational

power, increasing quantum system size and development towards fully fault-tolerant quantum systems must occur. Although encouraging, current findings cannot definitively prove quantum advantage in drug discovery, and future research should aim to find more conclusive evidence suggesting this advantage. Moreover, efforts to lower the costs of quantum computing as a whole and to make it more accessible for all must be taken as well. In February 2025, IQM launched a 5-qubit affordable quantum computer primarily for educational and research purposes [13], demonstrating that affordable quantum computers are attainable in the near future. Quantum computing for industry use is also seeing a shift towards obtainability: accessible cloud-based services for a much cheaper price than purchasing specialized hardware have the potential to revolutionize the field entirely [30].

Conclusion:

For the first time, a quantum classical hybrid algorithm was used to identify candidates for KRAS inhibitors, suggesting a promising avenue of future research and development that could greatly improve KRAS inhibitor research, cancer research, and drug discovery as a whole. In the short term, increases in system size will not enhance the performance of variational algorithms such as the one used in the experiment. Such development will only make substantial progress in the future, when we reach the MegaQuOP and FTQC eras of quantum computing.

By optimizing the drug design process using quantum computing, more KRAS inhibitors can be discovered and developed than previously done before, which could in turn lead to the development of different types of cancer remedies at a quicker rate.

There also exist many economic barriers-to-entry with integrating quantum technology in drug discovery. Many nations and institutions will not be able to access quantum technologies due to their immense costs to maintain, resulting in an uneven distribution of wealth. Furthermore, the lack of qualified workers to work the highly specialized jobs associated with quantum technology combined with the growing demand of such work presents a significant challenge to the future of quantum computing research.

Implications for future research includes further investigation into the mechanisms of actions of the two most recently discovered KRAS candidates. Developments towards fully fault-tolerant quantum computers so that quantum system size can be increased is a promising avenue of future research, and is a considerable step towards establishing conclusive quantum advantage in the field of drug discovery. However, we must also strive for lowering costs of maintenance and research for quantum computers to make them more accessible and allow for a larger population to be able to make advancements in the field.

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