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Case Study

Use of Quantum Computers with AI Integration for Drug Discovery

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A B S T R A C T

The merging of artificial intelligence and quantum computing could be recognised as a revolutionising method in the field of drug discovery. The traditional process of drug discovery has been considered as expensive, consisting of much more human power and also time-consuming. Currently AI is being used to detect drugs. But the main need for today's world is to carry out these processes at a fast pace and with precision. Hence, Quantum computing could be proven to be a helping hand for AI, which would not only make the procedure faster but also come out with phenomena which are unknown to mankind. The research paper revolves around the topic and tries to point out the significance of this combination. The paper discusses the people's understanding of this topic and their responses on the survey related to the topic. The paper tries to represent research based on surveys of 2 kinds i.e. the information technology and pharmaceutical field. Gathering responses from both the fields and what they think about this technology and how much they think it would be favourable in the coming future.

Keywords: Quantum Computing, Artificial Intelligence (AI), Drug Discovery,Machine Learning (ML), Molecular Simulation

Introduction

The drug discovery phase consists of 4 main phases:

- **Early Drug Discovery:** This stage works on the screening for potentially suitable compounds, research and requirements needed for the process. AI and machine Learning algorithms are also used in this stage.
- **Pre-Clinical Phase:** In this stage, the drugs are tested in the laboratory and animals.
- **Clinical Phases:** Clinical phases involves volunteer testing, testing for the side effects, etc.
- **Regulatory Approval:** Once the testing phases are completed, the drugs need to get approved by the National Regulatory Authority before launching it into the market.

All these phases require money, time, and living organisms for testing. A typical drug discovery process can take up to 13 years and the ratio for a drug to successfully make it to the approval stage is 1:5000. A new drug discovery can cost around $2.6 billion. Hence, considering the grueling and time consuming and danger to animals, the process could be done in a more secured, high-outcome giving procedure by the use of quantum computing. As quantum computing have the ability for simulation, they are also considered to be many times faster than supercomputers.[1-3]

AI in Drug Discovery

Artificial intelligence has been proved to be beneficial in many fields, but in pharmaceutics it is mainly used for drug discovery, formulations and testing. AI algorithms also analyse gene and biological data to predict drug interaction.

Procedures in which AI is useful are:

- Target identification,
- Compound shortlisting, Establish relationships between compounds and their biological activities.
- Fault detection
- Structure building

Some of the AI tools are:

- **DeepChem:** An open-source library for drug modelling and property prediction
- **RDkit:** An open-source library for substructure searching and molecular feature extraction.
- **GraphConv:** Effective deep learning model for analysing molecular properties.
- **Autodock Vina:** Docking software which uses machine learning tools to predict the efficiency of a molecule binding to a protein structure.
- **SMILES transformer:** A molecule structure developer tool.[2,5]

Quantum Computers (Quantum Computing)

Quantum computers have the capability to process large and complex problems and solve them at exceptional speed. It makes use of quantum properties and states subatomic particles to store information. It works on the principle of the relative nature of quantum particles. The behaviour of these particles is not the same as the objects in our surroundings. They possess extraordinary behaviour to be present in more than one state at a given time also called superposition.

- Spinning of electrons, which is believed to be in more than one direction at a given point of time.
- Wave and particle nature of light.

These states of the particles are in relation with the state of the other particle around them. For Eg. Electrons have a dual spinning nature, i.e. they rotate in an upward as well as in downward direction at the same time. But we consider 2 electrons in a relative state with each other, which is called "quantum entanglement". Then if 1 electron, has upward spin, then the other electron will always have an upward spin, and if we separate these 2 electrons from each other, keeping them 100 light years away from each other. Anyhow, if we could know the spin of the 1st electron then we could also know the spin of the 2nd electron, which is 100 light years away.[3,4]

This information transferred at more speed than the speed of light itself. Thus, this is how quantum computers work. They use the state of the subatomic particles, like electrons and protons, to store and transfer information, making them massively faster than any other device and machine existing till date.

But with such features come some barriers, which are cost and stability as quantum computers require operate at sub-zero temperatures, and we have very little knowledge about how to operate these machines; hence, development and maintenance of these machines is also a barrier.[6-10]

Results And Discussion

Application to SARS-CoV-2 Vaccine Development When the SARS-CoV-2 bacterium, being the cause for the current COVID-19 pandemic, stood in the Wuhan region of China at the turn of the year 2019, no one even kept having foreseen what would happen. Through January 2020, China accepted original confinement in isolation measures, moving almost a billion folk. To many in the experimental and healing societies, it quickly became apparent that a post-COVID-19 experience would just include a few in the way of additional doses of the vaccine program. A significant challenge to realising this, however, is that the quicker a cure has always occurred, the mumps vaccine in 1967, took 4 years.

Vaccine development is a difficult process, taking about 10-15 years approximately to realise. Traditionally, an additional dose of vaccine is achieved by making use of inactivated viruses or by making use of a live weakened bacterium that has existed and developed in education to manage far less hostile bacteria. Once inoculated, accompanying vaccines established either of these approaches; our own B containers combine and store antibodies against the proteins meant on the surfaces of growing capsules so that we can climb an adjusting immune response as long as we encounter a live report of the bacterium. However, the skilled are few security concerns at this moment approach for COVID-19, likely the short time restraint what side-belongings from live weakened viruses can delay to attack By intervening in summertime, Moderna and Pfizer had settled themselves as the leaders in the race for cure growth by cultivating a COVID-19 cure. Both associations were more the only ones to take the mRNA cure approach, issuing the beginning Phase I/II clinical trial dossier on July 14th for Moderna and on August 12th for Pfizer. Although sample sizes were small—as they usually are in early chapter dispassionate trials—the results manifested hopeful security measures and antitoxin results against the spike protein from those the who caught the cure.[11,12]

AIML algorithms and models used:

- **Network-Based Algorithms:** To predict probable epitopes, these algorithms utilise techniques such as deep affecting animate nerve organs networks, slope-pushing decision timbers, and pretended affecting animate nerve organs networks.
- **Expression-Based Algorithms:** Expression-based algorithms play a crucial role in the cure happening, since they improve the immunogenicity and expression

of the cure by strengthening the order to make it more effective and secure.

- **Integrated Docking Simulation Algorithms:** A useful system to predict by which mechanism ligands will interact with subsequent target proteins seeks to apply coupled binding imitation algorithms.

The FDA grants danger use permission to two mRNA COVID-19 vaccines, the Pfizer-BioNTech and the Moderna COVID-19 vaccines, in late 2020. Because skill is an essential need for COVID-19 vaccines and the FDA's cure authorisation process can take months to years, the FDA first presents crisis use permission to COVID-19 vaccines established with less dossier than is usually necessary. The dossier has to prove that the vaccines are safe and efficient before the FDA can give danger use permission or authorisation. Vaccines have gone through — and touch search — thorough security monitoring.[5,8]

Literature Review

Integrating quantum computing with AI in medicinal research has ushered in the most exciting paradigm shift that is now on the verge of developing. Quantum computing provides unique possibilities for independentlyand precisely tracking multiple molecular interactions, while AI has developed the most useful methods for data analysis and predictive modelling. It dramatically reduces the time and costs required for classic drug discovery procedures because it is now possible to simultaneously screen candidate drugs, optimise molecular structure, and predict pharmacological properties quickly. The technique has been practically validated in the last few years and holds immense promise in completely revolutionising the development of new therapeutics. Convergence of quantum computing and AI in drug discovery has offered another approach to addressing some of the core complexities of molecular biology and pharmacology. The theory of superposition and entanglements involved in quantum computing makes processes on those platforms many times faster than processes on classical systems. This is quite suitable for the accurate simulation of molecular interactions, optimisation of chemical structures, and predicting the behaviour of drug candidates. Along with this, AI has performed quite a number of jobs.[6]

Methodology

Survey Design

The study was carried out by designing surveys for people belonging to 2 different kinds of fields: IT and medical (Pharmacy). The questions were MCQ based on people's understanding of the effectiveness of AI, in pharmacy and how much quantum computers could be effective if paired with AI considering the features and abilities of a quantum computer

Data Collection Process

The survey form was distributed to people belonging to the respective field via social media platforms like Whatsapp. User data was no collected for this survey, and only their responses were taken into consideration. A short description of AI and quantum computers was provided in the survey form for people to understand about the research and help them respond effectively.

Individual Selection

The one major benefit that the survey was that was it was collecting insights from people having knowledge about the respective field. Not completely, but everyone somehow had knowledge about AI and the medicine generation process. About quantum computers, there was a need to add information about what they are and how they work, as it is a topic about which not many people are aware, but attaching the description did help the responders and thereafter they participated in the survey procedure

Findings

Survey 1 Designed for people in the IT field

Use of Advanced technology in medicines

Advanced technology like AI, ML, supercomputers, quantum computers, etc. can be proven for a great cause. For the medicinal field of91.4% people think that it would be of great help (fig 1).

Reliance on computers for speed

34.3% of people completely showed their complete trust in the computers and machines, while 57.1% of people asked for proof and assurance (fig 2).

Current Challenges

About the major challenges shortlisted for traditional drug discovery, 60% people said that it is time-consuming, 22.9% of people claimed it to be very expensive and 17.1% found the lack of research and knowledge to be the main concern (Fig 3).

Survey 2 Designed for people in the medical field.

Use of AI with integration of quantum computers in drug discovery

Fig 4 Quantum computers with AI integration81.9% of people significantly agree that it would be beneficial in the field, while 18.2% had a neutral take on this (fig 4).

Areas AI is useful in

Fig 5 AI use in medicine generation Among many significant processes in drug discovery and generation, a majority of the people found it most useful in the prediction of compound interaction and their side effects. A large portion believed it to be useful for analytics purposes. Some claimed

its usefulness in a very important and controversial phase, i.e., clinical trials that are being conducted on animals, and some said that it would speed up the overall process (fig 5).

Trust on AI

The results here came out similar to the previous survey. People belonging to the medical field too majorly believe that AI can't be trusted blindly even if it has come to an outcome using a powerful tool like a quantum computer(fig 6).

Concerns on use of AI for drug discovery

Most people found that over-reliance on machines could be a concern, some voted for lack of transparency, and some believed that machines are not as ethically advanced as humans; hence, that could be a slight drawback (fig 7).

Replacement for humans?

18.2% of responders consider that humans are irreplaceable, which is true because no matter how advanced technology may get, human involvement would always be required (fig 8).

Interest

Asking about the interest, the majority said it to be of great relevance to the medical field and an interesting topic to know about (fig 9).

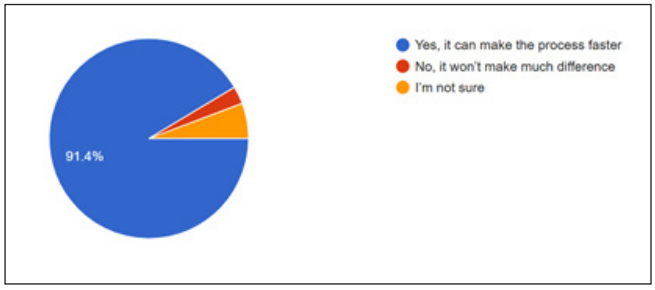

Figure 1.Advanced Technology in Drug Discovery Reflecting How Quantum Computers and Ai Can Together Help in Screening And Modelling

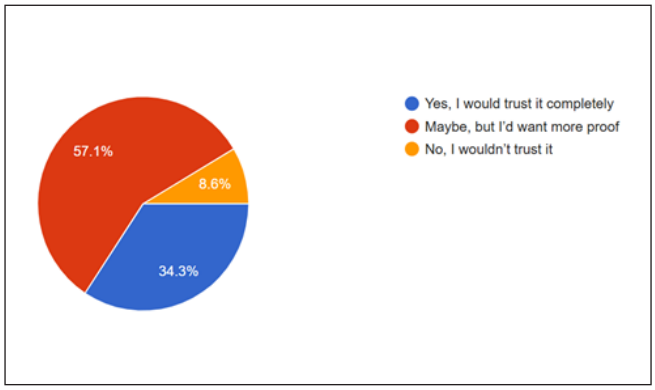

Figure 2.Shows Trust for Dependency on Computers

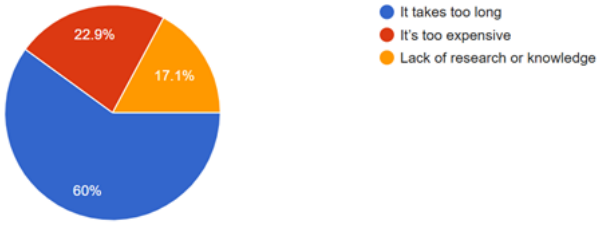

Figure 3.Illustrates the Challenges in Drug Industries

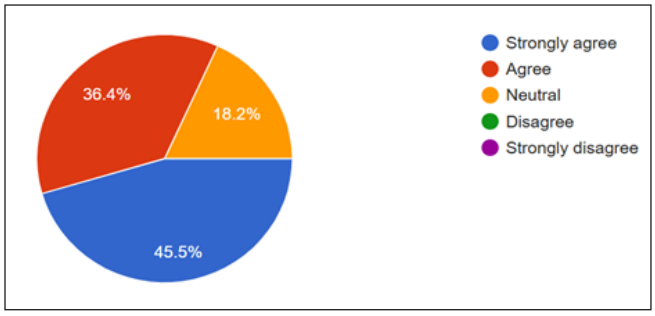

Figure 4.Quantum Computers with AI integration

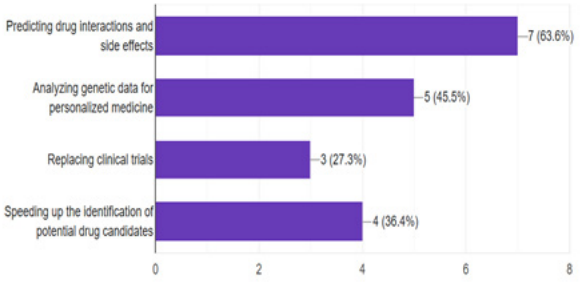

Figure 5.AI use in medicine generation

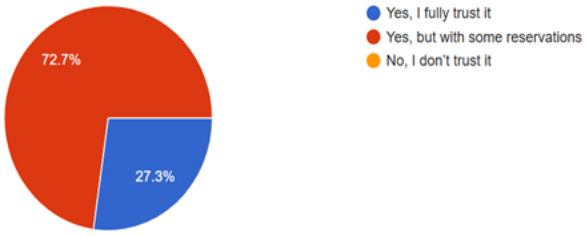

Figure 6.Reliability over Artificial Intelligence

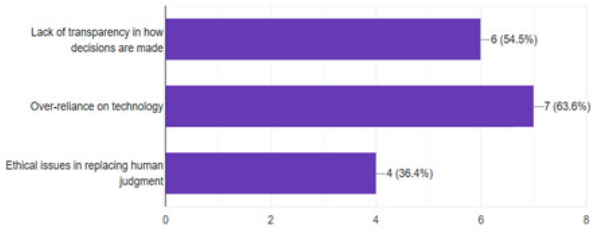

Figure 7.Problems with Using Ai

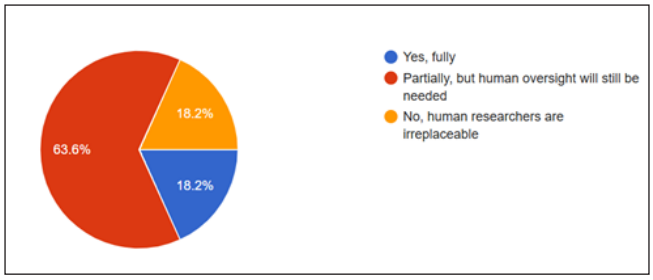

Figure 8.Are Humans Replaceable?

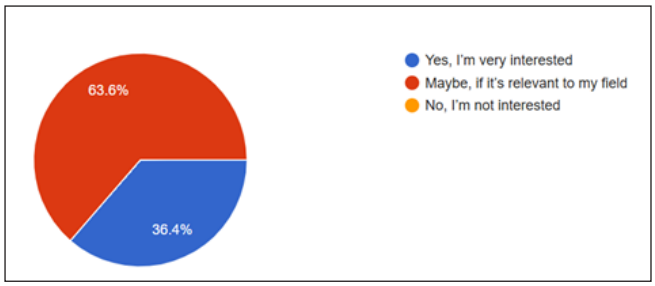

Figure 9.Keen Interest in the Topic

Outcomes

The survey for the research proved to be very useful in gathering insights and conclusive decisions regarding what people think about this newly emerging technology. Not only did people participate willingly, but they also encouraged others in the process.

We must the overall outcome one by one:

- **Technology in the medical field:** People do believe that involvement of technology is already proving to be beneficial and effectively lowers the burden on researchers and developers. [Fig. 4]
- **Relying on machines for research:** Computers are fast, and some of them did say that it made the process faster, but the majority think that getting the proof would increase their trust in the outcome. [Fig. 1]
- **Challenges:** Challenges and concerns in the traditional way in the time-consuming, high-cost and lack of knowledge. [Fig. 3]
- **AI withquantum computing:** The majority of the responders voted it to be beneficial, as it helps to bring insights and make researchers understand molecular interactions in a new way. [Fig. 6]
- **Useful areas:** Predicting molecular interactions and what would be their side effects could be considered as the top useful thing. Other than that, analysing the genetic data for personalised medicine use. Also, it takes thousands of drug samples, out of which 1 drug gets to the approval phase. Hence, AI can help create sample conditions, and quantum computing can help in simulation. Most importantly, animals are used in clinical trials. it is a debatable topic, but AI could greatly help in creating a similar environment, hence proving their significance. [Fig. 2]
- **Trusting AI:** Though AI is beneficial people always had their take on it to see to it that machine- suggested results must not be trusted blindly. [Fig. 5]
- **AI replacement for humans:** AI replacing humans is always a part of every technology conversations, and hence people say that even ifmachines provide us with solutions; humans must verify and clarify it before using it. [Fig.7, Fig. 8]

Hence, the overall outcome was that there are major concerns and drawbacks in the traditional way of the drug discovery process, like time, cost, and efficiency, etc. hence, people do believe that this pairing of artificial intelligence and machine learning with the extraordinary speed of quantum computers is and will be truly beneficial in areas like sampling, simulation, trails, etc., but they could not be trusted blindly and completely, claiming that human involvement would always be required.[7,8]

Conclusion

This research paper tries to discuss the problems with the typical and traditional way of medicinal research and discovery and shares the advantages of the topic. Hence, we could conclude that quantum computers with AI are more efficient than only using AI as a tool. Quantum computers are said to be 1000 times faster than traditional computers. They operate at a subatomic level and require a high investment to build one. But the outcomes and results they provide make the machines worthy of their pricing. They are very beneficial for simulations like molecular modelling, protein folding and agent and target pairing mechanisms. But behind the benefits of these admiring advantages, they have a few flaws, like, quantum computing is still in the very early stage of development; it still will take us years to reach at a stage about which this research paper talks;, it still requires stability and more research; and it would be working with the integration of AI, which will be needed for data sampling on which the quantum computers would make their decisions, on, so these data, as we know, will be collected from our very own history and sometimes it may happen that it does not come out with the correct result. Hence, human intervention will always be required in such cases. [Fig. 9]

Hence, creating a balanced, steady interaction between the quantum computers, AI and humans will always be the required factor.

References

1. The drug discovery process: What is it and its major steps? [Internet]. BioBide Blog. [cited 2025 June 24]. Available from: https://blog.biobide.com/the-drug-discovery-process
2. Vora LK, Gholap AD, Jetha K, Thakur RRS, Solanki HK,

Chavda VP. Artificial Intelligence in Pharmaceutical Technology and Drug Delivery Design. Pharmaceutics. 2023;15(7):1916. Available from: https://doi.org/10.3390/pharmaceutics15071916
3. Shearer D. Quantum Features - NQCC [Internet]. National Quantum Computing Centre; 2023 Aug 23 [cited 2025 Jun 24]. Available from: https://www.nqcc.ac.uk/quantum-features/
4. Making quantum computers with spin qubits – QuTech Blog [Internet]. 2018 Apr 20 [cited 2025 Jun 24]. Available from: https://blog.qutech.nl/2018/04/20/making-quantum-computers-with-spin-qubits/
5. Ghosh A, Larrondo-Petrie MM, Pavlovic M. Revolutionizing Vaccine Development for COVID-19: A Review of AI-Based Approaches. Information. 2023;14(12):665. Available from: https://doi.org/10.3390/info14120665
6. Evers M, Heid A, Ostojic I. Pharma's digital Rx: Quantum computing in drug research and development [Internet]. McKinsey & Company; 2021 Jun 18 [cited 2025 Jun 24]. Available from: https://www.mckinsey.com/industries/life-sciences/our-insights/pharmas-digital-rx-quantum-computing-in-drug-research-and-development
7. [7] King I. AI, energy and medicine: breakthroughs that will shape the future [Internet]. The Times; 2024 Dec 20 [cited 2025 Jun 24]. Available from: https://www.thetimes.com/business-money/economics/article/ai-energy-and-medicine-breakthroughs-that-will-shape-the-future-mcm860q35
8. Raza MA, Aziz S, Noreen M, Saeed A, Anjum I, Ahmed M, et al. Artificial Intelligence (AI) in Pharmacy: An Overview of Innovations. Innov Pharm. 2022;13(2):13. Available from: https://doi.org/10.24926/iip.v13i2.4839
9. Khullar D. How A.I. Teaches Machines to Discover Drugs [Internet]. The New Yorker; 2024 Sep 2 [cited 2025 June 24]. Available from: https://www.newyorker.com/magazine/2024/09/09/how-machines-learned-to-discover-drugs
10. Swayne M. What Are The Remaining Challenges of Quantum Computing? [Internet]. The Quantum Insider; 2024 Apr 21 [cited 2025 Jun 24]. Available from: https://thequantuminsider.com/2023/03/24/quantum-computing-challenges/
11. History of COVID-19: Outbreaks and Vaccine Timeline [Internet]. Mayo Clinic. [cited 2025 Jun 24]. Available from: https://www.mayoclinic.org/diseases-conditions/history-disease-outbreaks-vaccine-timeline/covid-19
12. Brothers W. A Timeline of COVID-19 Vaccine Development [Internet]. BioSpace; 2021 Dec 28 [cited 2025 Jun 24]. Available from: https://www.biospace.com/a-timeline-of-covid-19-vaccine-development