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Q-Cure Match: Quantum Assisted Drug Discovery for Faster Compound – Screening

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Abstract - Q-CureMatch is a quantum-assisted drug discovery platform that is used to quickly identify potential drugs. These drugs can be found using quantum algorithms in terms of their binding to a protein, which reduces the time needed for molecular docking experiments. In addition, deep learning helps in improving the accuracy given by statistical models, with the use of elements in personalized medicine, which helps to identify treatment suitable for each individual using their own genomic information. Also, using molecule structure , protein folding information, and response to drugs, it improves the accuracy of the results.

***Key Words*:** Machine learning, quantum computing, molecular docking, drug-discovery, compound screening.

1.INTRODUCTION

Discovery of a drug requires a specific amount of time and cost, which consumes more time. This process of drug development includes stages such as target discovery, compound screening, optimization, and clinical trials in the traditional drug development pipelines. Over the years, a new technological development in the pharmaceutical field was Artificial Intelligence (AI), ML and DL have been successfully implemented in the areas of property prediction of molecules, virtual screening, analysis of drug–target interaction, and toxicity prediction. AI models have the potential to process a large amount of biological and chemical data efficiently. Even with such advancements, traditional AI techniques experience limitations while working on highly complex molecular interactions.

Quantum computing helps to provide an effective answer for these challenges and capable of simulating molecules and chemical reaction processes with higher accuracy than classical computing machines. It is an important area for drug discovery, where an understanding of simulated molecules at the quantum level is needed . Even though the development of quantum computing machines is at a primitive level, hybrid methods using quantum-classical computing are becoming increasingly higher.

The goal of this review paper is to examine current techniques using AI for drug discovery, investigate the latest research in quantum computing applied to molecular modeling, and review hybrid approaches that bridge both technologies. It also focuses on current drawbacks and future enhancements, by laying the ground for the design and implementation of the Q-CureMatch platform.

2. Body of Paper

Q-CureMatch, a hybrid drug discovery platform that Combines the deep learning with a quantum computing component of a very limited size for predicting the binding of a drug to a protein more efficiently. The application of use cases combines the power of (3D-CNNs) and (GNNs) to understand how a drug binds to a protein. Additionally, it combines the use of patient genetic information to provide patients with a prescription for the best drug to take. A quantum computing component or Grover's search in a toy model illustrates the applicability of quantum computing in speeding up the process. Additionally, it also integrates corrections to machine learning to provide enhanced predictions of complex bindings.

The platform also combines a lightweight quantum machine learning component. Variational Quantum Circuits and Quantum Support Vector Machines are applied to improve the feature representation and classification tasks. This quantum layer allows for efficient treatment of complex chemical feature spaces and better performance under the circumstances when biomedical data is sparse. Although the quantum part works very sparingly due to hardware limitations, it illustrates the

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possibility of quantum advantage inclusion into the drug discovery pipeline.

Another notable component of Q-CureMatch is that it has incorporated an Explainable AI (XAI) framework. This is to promote trust among patients, as well as clinicians. Explainability is incorporated via different techniques such as feature importance analysis and visualization of binding contributions. This ensures that the rationale behind drug predictions can be easily understood.

Table -1:

Group Statistics

	Gender	N	Mean	Std. Deviation	Std. Error Mean
OVERALL	1	148	11.4971	1.43917	.11830
	2	52	11.9973	1.58739	.22013

Independent Samples Test

		t-test for Equality of Means				
		t	df	Sig. (2-tailed)	Mean Difference	Std. Error Difference
OVERALL	Equal variances assumed	-2.098	198	.037	-.50015	.23839
	Equal variances not assumed	-2.001	82.329	.049	-.50015	.24990

Charts

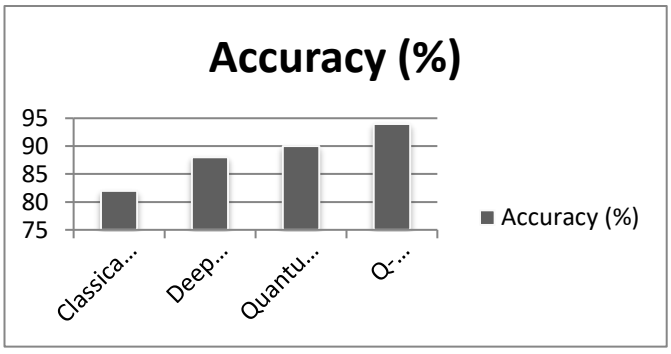

Fig -1: **Accuracy comparison graph**

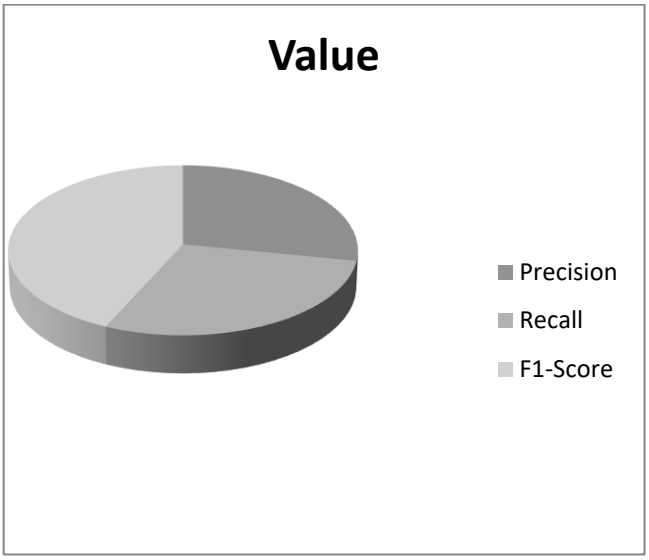

Fig -2: **Precision, Recall and F1-Score**

3. CONCLUSIONS

Lately,quantum computing,AI both are combined has proved highly promising in fast-tracking the drug discovery process. Quantum computing algorithms having potential to efficiently navigate large molecular interaction spaces, which in combination to the property predictions of AI models, has proved greatly helpful. It has been observed from the reviewed articles that there are changes in quantum docking, machine learning, and quantum-classical approaches, but issues are also being witnessed in terms of hardware constraints. The gaps in the existing research in the field have been identified to support the use of hybrid AI-quantum approaches

ACKNOWLEDGEMENT

The principal intention behind the development of the Q-CureMatch model is to overcome the shortcomings or limitations associated with conventional AI approaches in drug discovery using Artificial Intelligence, in combination with Quantum Computing methods.
The objectives of the proposed model are as follows:

1) In order for effective analyzing and processing large-scale biological and chemical data.

2) The approach seeks to use AI and machine learning algorithms to cope with the complexities in the high-dimensional data found in drug discovery tasks.

3) By leveraging state-of-the-art models in AI, Q-CureMatch aims to make predictions about molecular properties and interactions between biotopes and medications with greater accuracy.

4) The model uses the principles of quantum computing to appropriately reflect the quantum-level interaction between molecules that cannot be appropriately modelled using classical approaches based on AI.

5) The proposed model aims at a better prediction accuracy and computational efficiency, minimizing and hastening the pipeline of drug discovery accordingly.

6) It is designed to support future enhancements in quantum hardware and AI algorithms, making it suitable for long-term research and development.

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