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Hybrid Quantum-Classical Machine Learning Architectures for Accelerated Drug Discover

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Abstract: *Rapid drug development has been increasingly prevalent over the last ten years, and this trend, when combined with efficient regulatory approvals, has in large part been the driver for the rapid availability of innovative drugs to patients worldwide. This work presents a hybrid Variational Quantum Eigen seeker–Neural Network (VQE-NN) model, a single accelerated drug-solving device that leverages the benefits of both traditional and quantum computers. It performs drug class prediction and feature analysis based on the Kaggle Drug Classification dataset, which contains 2,000–3,000 records with categorical, textual, and numerical features. In data preprocessing, the researchers applied text normalization, tokenization, stemming, and TF-IDF-based feature extraction. The hybrid model presented consists of a VQE module for the optimization of molecular representations and a neural network for classification. In addition, the hyperparameters were carefully tuned to ensure the model learns efficiently and converges. The experimental results show the model's remarkable prediction capability as seen from an accuracy of 97.0%, precision of 96.3%, recall of 96.8%, F1-score of 96.5%, and an AUC of 0.9991. In the performance comparison, the VQE-NN model is claimed to be superior to the existing benchmarks, such as Generative RNN and Seq2Seq Autoencoder models. Besides, the research highlights the benefits of the model, which stem from using quantum entanglement and superposition, which allows for the identification of correlations in higher dimensions and offers a scalable, robust, and state-of-the-art framework for drug prediction.*

Keywords*:* Accelerated Drug Development, Hybrid-Quantum Classical Computing, Quantum-Machine Learning, Drug Discovery, Quantum Optimization

I. INTRODUCTION

A more conventional, all-encompassing view of health has long been the basis of drug research. Across the turn of the previous century, allopathic medicine became the norm in hospitals and clinics across the globe. Despite the effectiveness in battling illnesses brought about by this transition, the burden of high medication costs has been a drag on healthcare systems. Despite a wide variety of factors, including candidate-specific factors, the cost of developing and discovering new drugs has climbed substantially over the past few years [1]. In health and illness, biological systems provide a wealth of complicated information [2]. An abundance of "omics" and "smart" devices are currently measuring and mining this data at previously unseen levels. As the pharmaceutical industry strives to discover potential therapeutic hypotheses for drug development, the rise of high-throughput methods to biology and illness brings both obstacles and opportunity. The expedited review process for drug approval needs to be rigorous. It is only fair that trial participants be held to the same standards of beneficence and non-maleficence as the general public [3]. There are those who believe that expedited approval compromises safety and that it is anti-scientific and immoral to approve a medicine based on insignificant data.

Significant advancements in hardware and algorithms have allowed quantum computing to progress at a rapid pace in the past few years. These developments are bringing the commercial use of quantum computers closer to its inevitable arrival [4]. Many of these new devices may have potential uses in the exciting field of drug development [5]. This capability enables the description of chemical systems faster and more precisely using quantum simulation than traditional quantum chemistry methods. It is not a secret that the data patterns produced by quantum physics are both

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notoriously paradoxical. A typical similarity between classical ML methods, including deep neural networks, is that they are capable of identifying patterns in input data and extrapolating new data with the same patterns [6]. A new field of research known as hybrid quantum-classical machine learning (ML) combines classical neural networks with quantum variational circuits on noisy intermediate-scale quantum devices. Quantum Machine Learning (QML) is a novel approach that integrates ML with QC. It is a great chance for businesses and researchers to create ground-breaking discoveries and find effective solutions to complicated real-world issues, with a strong focus on practicality and better accuracy than traditional systems [7]. With QML, the community has more chances to discover, build, and link their ideas to various quantum stack levels.

Pharmaceutical companies are increasingly using ML and artificial intelligence (AI) to speed up drug discovery and development. The increasing digitization of pharmaceutical data opens up opportunities for, but also poses challenges to, the extraction of actionable insights for complex clinical problems [8]. ML algorithms enable predicting chemical, biological and physical properties of compounds consequently, the study becomes efficient. Thanks to the advances in computational sciences, AI, and, in particular, ML and DL, are now at the center of the industry and the field of academia, which has resulted in the development of data analytics, automated systems, and intelligent systems.

A. Motivation and Contributions of the Study

The conventional drug discovery methods are extremely slow, costly, and largely inefficient because the biological mechanisms are too complex, and the chemical search space is very large. Pharmaceutical research has been struggling to accurately predict drug effectiveness, safety, and interactions, despite advancements in digitization and computational techniques. AI and ML usage have significantly enhanced the data-driven decision-making process; however, classical computational models face issues with scalability and optimality in high-dimensional molecular data. When it comes to today's reality, quantum computing is trying to change everything. QML models are hybrid quantum-classical computers that use quantum features like entanglement and superposition to improve human capacity for pattern identification, chemical modelling, and prediction precision. The article is based on the development of an efficient, scalable, and precise drug discovery system through a hybrid quantum-classical strategy that does not only accelerate drug discovery and reduces the cost but also enhances potential therapeutic agents' discovery. The significant contributions that the research makes are expounded below:

- Utilized the Kaggle Drug Classification dataset containing 2,000–3,000 records with categorical, textual, and numerical features, providing comprehensive information on drug names, chemical properties, target conditions, and classes.
- Applied text normalization, text tokenization, and stemming to standardize textual data and prepare it for ML and quantum-classical modelling.
- Used TF-IDF to convert the pre-processed text into numerical features suitable for model training and analysis.
- Optimizes both quantum (ansatz type, qubits, depth, classical optimizer) and neural network parameters (layers, neurons, learning rate, regularization) for improved convergence and generalization.
- Developed a Hybrid Variational Quantum Eigen solver-Neural Network (VQE-NN) model that integrates quantum computing with classical optimization for accelerated drug prediction.
- Attained exceptional outcomes in terms of recall, accuracy, precision, F1-score, loss, and area under the curve (AUC), suggesting nearly flawless classification capabilities.

B. Novelty and Justification of the Study

To improve the speed and accuracy of drug discovery prediction, this study introduces a novel hybrid quantum-classical framework that blends classical neural networks with the Variational Quantum Eigen solver-Neural Network (VQE-NN). The framework under development employs quantum superposition, entanglement and parallelism in a quite different manner than the traditional ML models, in order to efficiently explore high-dimensional molecular spaces, and in order to explain the complex correlations in chemical data. The system can then converge faster, model interactions among molecular interactions more accurately, and make more predictions due to this integration. The research has

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been justified by the increasing need to scale and be accurate in computational procedures in drug discovery, which in most cases involve classical model that often has difficulty handling sophisticated biochemical associations. It is a radical solution because it involves quantum computing, the incorporation of classical learning, and advanced data pre-processing (TF-IDF), which is an efficient solution to the issue of drug recovery prediction being rapid and reliable in biomedical informatics.

C. Structure of the Study

The paper is organized as follows: Section II reviews related work on accelerated drug discovery. Section III describes the dataset, text pre-processing, feature vectorization, and the proposed Hybrid Quantum VQE-NN model. Section IV presents experimental results and compares performance with benchmark models. Section V concludes the study and suggests directions for future research.

II. LITERATURE REVIEW

This study is grounded in a thorough review and critical assessment of existing research on accelerated drug discovery, which informed the refinement of its objectives and guided the overall direction of the investigation. Table I summarizes recent studies on accelerated drug discovery, highlighting their objectives, methodologies, sources, relevance, and limitations.

Zhang, Li and Zandt (2020) Its goal is to connect Chinese and American clinical drug databases by bridging the gap between Rexnord, the International Rexnord Extension, and the Normalized Chinese Clinical Drug (NCCD) database are all part of the OHDSI research network. Findings showed that 2,247 (or 25.39%) NCCD semantic clinical medicines can be mapped to Rexnord, whereas 588 (or 6.64%) may be mapped to Rexnord Extension. At the constituent level, 99.6% of the top 1000 clinical medications in China are chemical pharmaceuticals, and they can all be mapped to Rexnord/Extension [9].

Ru et al. (2019) explored models using DNN to extract data on accidental drug use from social media. To create word-embedding characteristics, they analyzed medication evaluations shared on a WebMD patient forum using the word2vec algorithm. After collecting contextual information from drug-review postings, information-filtering tools, medical oncology, and medical expertise, they made adjustments and reconstructions to the convolutional neural network, long short-term memory network, and convolutional long short-term memory network. Using a standard dataset of 15714 words, the models were trained, fine-tuned, and evaluated. Out of this dataset, 447 (2.8%) described unintentional drug usage. On top of that, they benchmarked their DLNs against SVM, RF, and AdaBoost.M1 algorithms [10].

Rashid et al. (2019) presenting a drug prediction algorithm that aids patients in selecting the most appropriate medications to treat their specific ailments. To conduct preliminary data analysis for medication recommendations related to a user's symptoms, the MLLib Library of Apache Spark is utilized. The program takes into account the weather and the maps API from Google, in addition to the patients' past medical history, to determine the likelihood of adverse drug reactions and to help patients find local pharmacies that stock their medications [11].

Zylich et al. (2018) Provided techniques to enhance the creation of algorithms that match established rules, the standardization of reaction names, and the matching of drug names to enable the mining of safety data for interesting pharmaceutical combinations. They have developed a measure for medicine name matching. They were able to demonstrate that their method was effective with a sensitivity score of 0.855, which corresponds to 91% accuracy. They examined the impact of several response name standardization approaches on known-rule matching and found that using their approaches, Out of 4652 signals that were made, 427 rules were found; however, out of 3276 signals that were generated without their approaches, 61 rules were recognized [12].

Wang et al. (2018) they used ANTENNA to tackle a practical issue: finding new uses for existing medications in clinical settings where they have not been useful in the past. It was shown that the medication diazoxide, which is licensed by the FDA, may effectively kill cells of triple negative breast cancer (TNBC) with an IC50 value of 0.87 μM, as well as block several kinase genes that are relevant to many disorders, including cancer. Targeted therapy for TNBC is ineffective, making the illness fatal. Their findings demonstrate that big data analytics has had the ability to

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completely transform the pharmaceutical industry and lead to the creation of individualized therapies for TNBC [13]. Rachmani et al. (2018) depict the actions of leprosy patients when taking MDT medications over a long time by utilizing an apriority algorithm to mine connection rules between the timeliness of MDT visits to healthcare establishments. Starting on June 1, 2012, and ending on June 30, 2014, data were gathered from a cohort of 27 PHCs in the Pekalongan District that participated in a manual leprosy registry. The new labels for the range of dates between MDT collection attendances, which were transformed in this study, are on-time attendance (OTA) and on-time completion (OTC). An relationship between MDT 2 and MDT 3 is strongly related to leprosy patients' tardiness in completing treatment, as seen in both MB and PB patients [14].

A. Identified Gaps in Previous Studies

Current approaches often lack comprehensive integration across global drug databases and underutilize unstructured data from sources like social media. Personalized drug recommendation systems frequently overlook individual patient history, environmental factors, and real-time availability. Most of the current methods used to extract drug interactions are mainly rule-based and might miss newly combinations of drugs, while drug repurposing systems have a limitation in their scalability for various diseases. Moreover, research on patient adherence is mostly specific to a particular disease or region, and a great number of methods depend on manual curation, thus there is a demand for automated, scalable, and data-driven approaches that can speed up drug discovery.

Table: Recent Studies on Accelerated Drug Discovery using machine learning

Author	Study Focus	Source	Approach	Relevance to Accelerated Drug Discovery	Limitations
Zhang, Li & Zandt (2020)	Linking clinical drugs in China with USA and international standards	Database of Standardized Chinese Clinical Drugs (NCCD), RxNorm, and RxNorm Extension	Drug concept mapping across NCCD and RxNorm/OHDSI networks	Facilitates standardized drug identification across regions, aiding global drug efforts	Mapping is limited to available semantic data; incomplete coverage of all drugs
Ru et al. (2019)	Mining serendipitous drug usage from social media	WebMD patient forum (15,714 sentences)	Deep Neural Networks (CNN, LSTM, ConvLSTM) with Word2Vec embeddings; compared with SVM, Random Forest, AdaBoost	Identifies potential new drug uses and interactions, supporting accelerated drug discovery	Low prevalence of serendipitous cases (2.8%), potential bias in social media data
Rashid et al. (2019)	Personalized drug prediction for patients	Patient symptom data, historical drug responses, Google Maps	ML model using Apache Spark MLLib, considering side effects, weather, and drug availability	Supports timely and accurate drug recommendations, improving drug recovery efficiency	Requires integration of diverse real-time data; scalability issues
Zylich et al. (2018)	Medication combination high-fidelity rule mining	Drug safety reports	Sensitivity measure for assessment; rule mining with medication name matching, reaction standardization, and	Enables detection of safe and effective drug combinations, aiding optimized drug recovery	Limited to known drug rules; novel interactions may be missed

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			known-rule matching		
Wang et al. (2018)	Drug repurposing for new clinical indications	FDA-approved drug data, kinase gene targets	ANTENNA big data analytics framework	Accelerates identification of effective drugs for diseases like TNBC, reducing time to therapy	Validation limited to specific disease (TNBC); may not generalize
Rachmani et al. (2018)	Patient adherence to leprosy MDT treatment	Manual leprosy registry cohort (27 PHCs, 2012–2014)	Association rule mining (Apriori) to analyze on-time attendance and completion	Improves understanding of treatment adherence, supporting effective drug delivery	Focused on one disease and region; small dataset

III. RESEARCH FRAMEWORK

The drug classification technique outlined in the proposal is supported by a detailed drug classification dataset sourced from Kaggle. The data undergoes an initial stage of pre-processing where text normalization, tokenization, and stemming are carried out to standardize and improve the quality of text features. The next step involves using TF-IDF vectorization for feature extraction, which transforms the text input into numerical formats that ML can understand. There are two types of data: training and testing for classification, a hybrid model integrating Variational Quantum Eigen solver (VQE) and a Neural Network (VQE-NN) is used, and hyperparameter tuning is employed to boost the model's performance. Various performance metrics are employed to assess the model's effectiveness in determining the degree of categorization performance. Recall, accuracy, precision, loss, F1-score, and ROC analysis are all measures that fall into this category. A process flow diagram is shown in Figure 1.

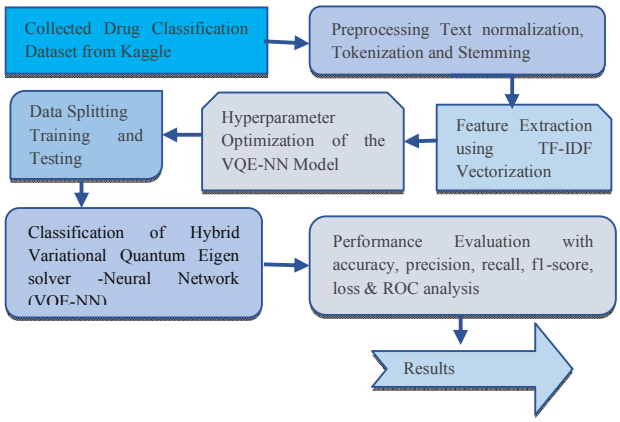

Fig. 1. Proposed Flowchart for Accelerated Drug Discovery

The following section explains the process shown in the proposed flowchart for Accelerated Drug Discovery.

A. Data Collection and Visualization

The study utilized the Kaggle Drug Classification dataset containing details of drug names, active ingredients, target diseases, chemical properties, and drug classes. With a size of about 2,000-3,000 records, the dataset contains categorical, textual, and a few numerical features, which is suitable for ML tasks such as the prediction of drug classes, feature analysis, and NLP-based extraction from chemical or textual descriptions. Table II presents the drug classification of the dataset.

Table 2: Drug Classification

Age	Sex	BP	Cholesterol	Na_to_K	Drug
23	F	HIGH	HIGH	25.355	DrugY

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47	M	LOW	HIGH	13.093	drugC
47	M	LOW	HIGH	10.114	drugC
28	F	NORMAL	HIGH	7.798	drugX
61	F	LOW	HIGH	18.043	DrugY

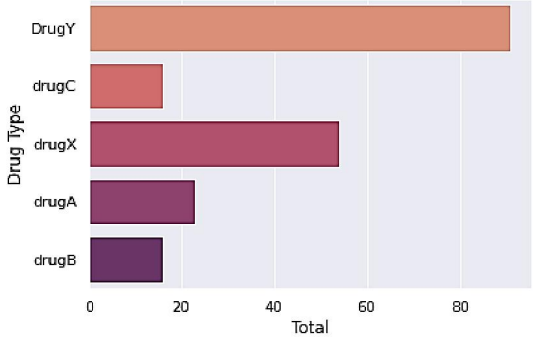

Fig. 2. Drug Type Distribution

Figure 2 depicts a horizontal bar chart illustrating the overall counts for five different drugs: Drug B, Drug A, Drug X, Drug C, and Drug Y. Drug Y is the one to have the most significant number of instances (90) and, therefore, ranks first. Besides that, the count for Drug X is almost half that of Drug Y (55), and thus, Drug X is in the second place. Meanwhile, the three drugs i.e., Drug A, Drug C, and Drug B with the values of 25, 18, and 15, respectively, have their total numbers considerably less than those of the first two drugs. A color gradient from dark purple (lowest) to light reddish-orange (highest) adds to the visual separation of the different drug types by color.

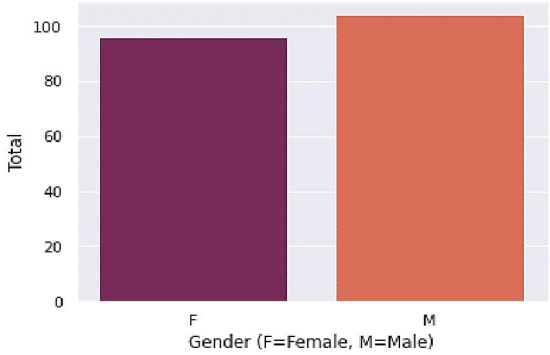

Fig. 3. Gender Distribution

Figure 3 illustrates the overall numbers for two genders: Female (F) and Male (M). The Males had a little more (105) than the Females (95), so the number of the two genders was almost equal, with just a little bit more males.

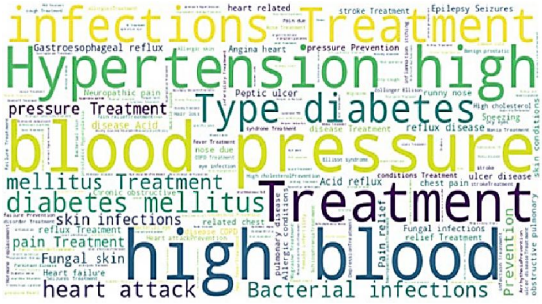

Fig. 4. Uses of Medicines

Figure 4 shows a word cloud that visually represents the frequency of medical conditions and associated terms in the dataset. The size of the words is proportional to their frequency, with the most frequent words being prominently

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displayed. These words include BLOOD pressure, Treatment, INFECTIONS, Hypertension, high blood pressure, and Type diabetes. The occurrence of terms like mellitus, heart attack, Acid reflux, and Epilepsy Seizures also suggests that the dataset is concentrated on chronic and infectious diseases that are common.

Fig. 5. Word Cloud of Different Observations

Figure 5 shows the word cloud reflecting the most frequently mentioned drug names and dosages. Some of the very visible names are Metformin 500mg, Metformin 1000mg, Telmisartan 40mg, Glimepiride 1mg/2mg, Montelukast, Amlodipine 5mg, and Metoprolol Succinate. The large stylized "W" letters in purple and green are part of the background. The fact that drugs such as Metformin, Glimepiride and Telmisartan are mentioned frequently should indicate that Priority was given to the treatment of long-term conditions including diabetes and high blood pressure.

B. Data Pre-processing

To ensure the accuracy and dependability of the analysis, data pre-treatment is a requisite step. Alternative keen procedures were used to prepare the data in the succeeding phases of work.

- **Text Normalization:** Text normalization was performed to bring about consistency and eliminate duplication by differences in cases and thus involved the transformation of all text data to lowercase. After removing the mean and standard deviation from the temperature data, Equation (1) is used to normalize the data.

$$T' = \frac{T - \text{mean}(T)}{\text{std}(T)} \qquad (1)$$

- **where, T:** original data or feature values; $\text{mean}(T)$: The **mean (average)** of all the values in T; $\text{std}(T)$: **standard deviation** of the values in T.
- **Text Tokenization:** The text was tokenized to make analysis easier and to allow for additional cleanup by dividing it into separate components. Because the main focus was on linguistic element analysis, special letters and numerals were removed so that the text could be fully examined.
- **Stemming:** In stemming, all of a word's possible forms are compressed into one common representation, the stem. To illustrate the point, the terms "presentation," "presented," and "presenting" might all be shortened to the single word "present."

Feature Extraction using Term-Frequency-Inverse Document Frequency (TF-IDF) Vectorization

The term "Term frequency (TF)" is described under the section titled "Term details." Words that appear too frequently in the collection of papers may be helpful for discriminating between those, but IDF and TF work together to reduce their impact [15]. IDF is calculated as follows in Equation (2):

$$\text{idf}_t = \frac{\log N}{df_t} \qquad (2)$$

where N is the total number of documents in a collection and df_t stands for the document frequency of word t, which is the count of documents in the collection that include t. Equation. (3) is used to compute the TF-IDF of a compound word:

$$\text{tf} - \text{idf}_{t,d} = \text{tf}_{t,d} \times idf_t \qquad (3)$$

As a result, TF-IDF for a t is high when t is included in a limited set of documents several times.

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C. Hyperparameter Optimization of VQE-based Neural Network

The hyperparameters of the VQE-based Neural Network were carefully optimized to ensure effective learning and convergence. For the neural network component, the number of layers was set to four, comprising an input layer, two hidden layers (Dense1: 128 neurons, Dense2: 64 neurons), and an output layer, with ReLU activations in hidden layers and Softmax or Sigmoid in the output layer, depending on the task. To train the model, used the Adam optimizer with the following parameters: 32 batches, 0.001 learning rate, and 30 epochs. To avoid overfitting, used regularization techniques like dropout (0.3) and L2 weight decay (1e-4). For the VQE component, the ansatz type, number of qubits, and depth were selected based on the problem Hamiltonian, while the classical optimizer (COBYLA, SPSA, or Adam) was tuned along with the maximum iterations (200–500) and convergence tolerance (1e-6). The initial parameters for the ansatz were either randomly initialized or specified according to the system's physical characteristics. Hyperparameter optimization involved iterative experimentation to balance accuracy, convergence speed, and model generalization. Table III as illustrates the hyperparameters of the hybrid models are as follows:

Table 3: shows certain hyperparameters of the Hybrid Model.

Model Hyperparameters		
Component	Hyperparameters	Values
Variational Quantum Eigensolver	Ansatz type	Hardware-efficient / UCCSD / Custom
	Number of qubits	Depends on Hamiltonian (e.g., 4–12 qubits)
	Ansatz depth (layers)	2–4
	Classical optimizer	COBYLA / SPSA / Adam
	Maximum iterations	200–500
Neural Network	Number of layers	4 (Input, 2 Hidden, Output)
	Neurons per layer	Input: depends on features, Dense1: 128, Dense2: 64, Output: depends on task
	Activation functions	Dense1 & Dense2: ReLU, Output: Softmax/Sigmoid
	Learning rate	0.001
	Batch size	32

E. Data Splitting

The extracted features are thereafter split in half lengthwise to serve as a training set and a test set, with a ratio of 80:20.

F. Proposed Hybrid Quantum Model's Classification

In this section, the proposed Hybrid VQE-NN model is used for Drug Discovery. The model is discussed below:

To determine the Hamiltonian's ground state, one may utilize the eigenvalue of a hybrid method called the Variational Quantum Eigen solution (VQE), which blends classical and quantum methodologies. One of the cornerstones of VQEs is the variational concept. Minimizing the anticipated value of the Hamiltonian for a parametric model state is an integral part of virtual quantum equations (VQEs) this expected value through parameter tuning with a classical optimizer [8].

The physical properties of the system may play a role in determining the ansatz state. The fact that the eigenvalue issue, this, as is well known, may be reformulated as an operator $\mathcal{H}$ represented observable is part of a variational issue on the Rayleigh distribution. In Equation (4), find the Ritz ratio that minimizes the eigenvector $|\psi>$which corresponds to the lowest eigenvalue.

$$\frac{<\psi|\mathcal{H}|\psi>}{<\psi|\psi>} \qquad (4)$$

By varying the experimental parameters in the preparation of $|\psi>$. At the termination of the algorithm [16], In the last set of experimental parameters that determine $|\psi>$, there is an easy way to save the prescription for eigenvector reconstruction. Neural networks are artificial models that aim to reproduce the brain's information processing capabilities. The network is constructed by interconnecting groups of neurons (nodes) that create an output layer, one or

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more hidden layers, and an input layer. The network is able to learn sophisticated, non-linear connections between inputs and outputs because each neuron employs an activation function and weighted connections to understand incoming data [17]. In order to train neural networks, optimization techniques like gradient descent are used to alter weights in a way that minimizes a loss function. These networks have several applications, including classification, regression, image recognition, and natural language processing (NLP).

G. Evaluation Metrics

The metrics that are used to evaluate metrics for the experiment's success: ROC analysis, recall rate, accuracy, precision, and F1-score.

The F1-score is formed by summing accuracy, which is defined as the percentage of samples that are properly categorized, and precision, which is defined as the proportion of positively predicted occurrences out of all instances predicted as positive, are related concepts in ML [18]. Evaluating a binary classifier's performance, it takes into account both loss and ROC analysis. Loss measures how well a model's predictions match the true values, as ROC illustrates the ratio of true positives to false positives over different thresholds. Its total discriminative ability is indicated by the Area Under the Curve (AUC). The formulas for the metrics are as follows in Equations (5)-(8):

$$Acc = \frac{TP+TN}{P+N} \quad (5)$$

$$Pre = \frac{TP}{TP+FP} \quad (6)$$

$$Rec = \frac{TP}{TP+FN} \quad (7)$$

$$F1 = \frac{2\times precision\times recall}{precision+recall} \quad (8)$$

This is probably how the confusion matrix's parameters are defined: TP stands for the total number of correctly detected positive instances. When it comes to positive examples, the model gets them right, while TN represents how many times it gets the negative prediction right. The model accurately identifies negative situations, and FP represents the number of times it incorrectly predicts positive outcomes. The model may have incorrectly predicted a negative class in certain FN occurrences, even if that is not necessarily the case. Even though the actual class is positive, the model predicts that it is negative.

IV. PREDICTED EXPERIMENTAL RESULTS

The experimental setup employed pre-2020 hybrid quantum–classical frameworks. Classical tasks ran on an Intel Core i7 system with 16 GB RAM and an NVIDIA GTX 1080 Ti GPU under Ubuntu 18.04, while quantum experiments used IBM Q Experience (5–16 qubits) and Rigetti Forest SDK. Software included Python 3.7, Qiskit 0.14, Cirq 0.6, PennyLane 0.6, scikit-learn 0.22, TensorFlow 1.14, PyTorch 1.3, and RDKit 2019.03. Qiskit Aer simulators handled large-scale runs, with select circuits tested on IBM Q hardware for noise evaluation. Table IV displays the outcomes of the performance evaluation for the hybrid model that was suggested, which integrates the Variational Quantum Eigensolver-Neural Network (VQE-NN) for accelerated drug Discovery. The model exhibits powerful prediction power as it reaches an accuracy of 97.0%, thus suggesting that it is highly correct overall in its classification. The 96.3% accuracy rate shows that the model is doing a good job of reducing false positives, while the 96.8% recall rate shows that it can detect relevant cases rather well. Additionally, the 96.5% F1-score value is a clear indication that the model has maintained a well-rounded compromise between recall and precision, thereby validating a robust and dependable hybrid model for optimizing medication predictions.

Table 4: Performance Evaluation of the Hybrid Proposed Model for Accelerated Drug prediction

METRICS	VARIATIONAL QUANTUM EIGENSOLVER-NEURAL NETWORK (VQE-NN)
ACCURACY	97.0
PRECISION	96.3
RECALL	96.8
F1-SCORE	96.5

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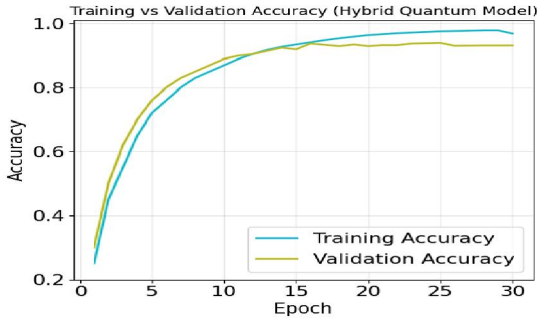

Fig. 6. Training and Validation Accuracy of the Model

Figure 6 shows the Hybrid Quantum Model's training vs validation accuracy across 30 epochs. Both accuracies are in a fast upward trend from 0.25 to more than 0.90 during the first 10–15 epochs and then they are getting close to the plateau. To be more precise, the training accuracy is still going up by a very small margin and its value is very close to 1.0, whereas the validation accuracy reaches about 0.97 and stays constant, a little below the training curve, thus suggesting that there is a slight overfitting in the last epochs.

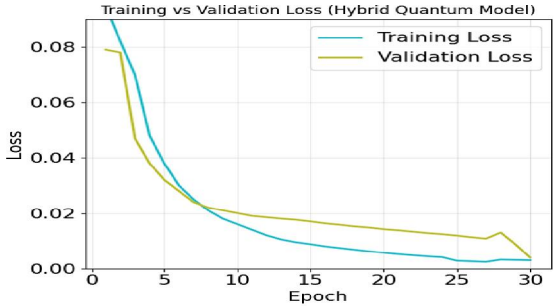

Fig. 7. Training and Validation Loss of the Model

The loss for the Hybrid Quantum Model during training and validation across 30 epochs is shown in Figure 7. After about 5-10 epochs, the losses are already less than 0.08, and then they gradually stabilize. The training loss is always a bit lower than the validation loss, and it goes down to almost zero at the end, whereas the validation loss stays at a low level with some minor fluctuations, thus suggesting slight overfitting.

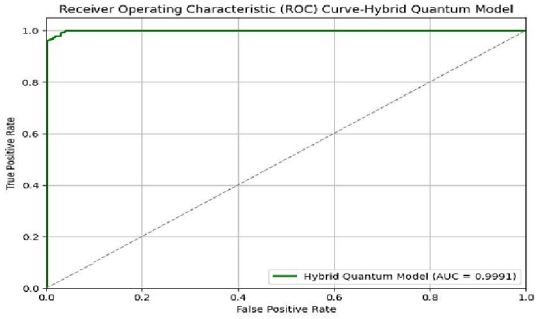

Fig. 8. ROC Curve of VQE-NN

Figure 8 illustrates the ROC for a Hybrid Quantum Model, a graph showing the ratio of TP to FP. The model shows extraordinarily good classification performance as the curve is almost on the top-left border. In fact, this is supported by a very close to perfect AUC of 0.9991, which is a near-perfect score, and the model is thus extremely efficient in differentiating the predicted classes and hence its performance is way better than that of a random classifier (dashed line, AUC of 0.5).

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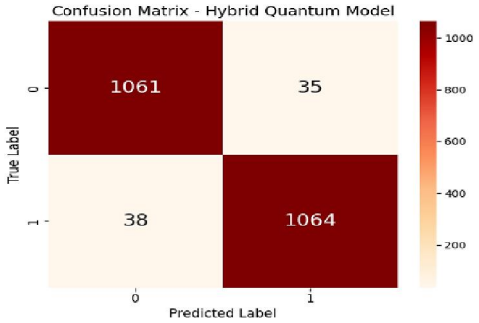

Fig. 9.Confusion Matrix of the VQE-NN

Figure 9 represents the Confusion Matrix for the Hybrid Quantum Model, showing the model's ability to classify data for classes 0 and 1. 1061 instances of class 0 (True Negatives) and 1064 cases of class 1 (True Positives) have been accurately detected by the model, demonstrating its high level of accuracy. The number of misclassifications is quite low, with just 35 FP (class 0 projected as 1) and 38 FN (class 1 forecasted as 0). A balanced matrix like this shows that the model can function properly and is stable for both classes.

A. Comparative Analysis

Table V exhibits a comparative study of performance between current benchmark models and the newly introduced model in the scenario of prediction for drug discovery acceleration. It illustrates the accuracy obtained by three models: the Generative Recurrent Neural Network (RNN) model, which achieves an accuracy of 86%; the Sequence-to-Sequence Autoencoder (Seq2Seq AE) model, whose accuracy is notably higher at 96.2%; and the proposed Variational Quantum Eigensolver-Neural Network (VQE-NN) model that goes beyond both the benchmarks with an accuracy of 97.0%. This comparison is a clear indication of the superior performance of the VQE-NN-based method, which is an efficient way of increasing predictive accuracy and thus making drug recovery processes more efficient.

Table 5: Performance Comparison of Benchmarking Models with Proposed Models for Accelerated Drug Discovery prediction

Models	**Accuracy**
Generative RNN [19]	86%
Seq2Seq AE [20]	96.2
VQE-NN	97.0

The benefits of the Proposed VQE-NN are shown in Table VI below.

Table 6: Advantages of the VQE-NN Model

Advantage Type	**Key Advantages of the VQE-NN Model**
Quantum Advantages	Exploits **quantum superposition and entanglement** to explore exponentially large solution spaces.
	Enables **rapid optimization of complex molecular structures and interactions**
	Quantum parallelism enhances identification of optimal drug candidates.
	Improves predictive accuracy and robustness beyond classical capabilities.
	Captures **subtle correlations in high-dimensional chemical data.**
	Provides a **scalable and high-fidelity approach** for predicting drug.
Hybrid Advantages	A hybrid quantum-classical algorithm combines the strengths of quantum circuits
	Classical components handle **data preprocessing, optimization, and parameter updates**, reducing computational overhead.
	Enables **faster convergence** and **improved scalability** compared to purely classical or quantum models.

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	Allows **flexible model design**, using quantum resources where most beneficial.
	Achieves **enhanced predictive accuracy, robustness, and reliability**.
	Maximizes **strengths of both paradigms**, achieving **state-of-the-art performance** in drug discovery prediction.

V. CONCLUSION AND FUTURE WORK

In comparison to conventional therapy without group and those who decline or discontinue treatment, individuals undergoing drug use disorder group treatment often show greater progress on usual outcome measures. In conclusion, this study shows that an efficient method for making quick predictions about new drugs using the Kaggle Drug Classification dataset is the Variational Quantum Eigen solver-Neural Network (VQE-NN), which combines quantum and classical approaches. The model put forward, which is a combination of quantum computing and classical optimization, has accomplished a phenomenal performance, including a 97.0% accuracy rate, a very high precision, recall, F1-score, and almost perfect discriminative ability, thus going beyond the benchmark models. The research shows that data preparation, feature extraction, and visualization are crucial steps in making models more reliable. Predicting drugs in a method that is efficient, accurate, and resilient is made possible by hybrid quantum models.

For future work, the approach may be applied to sizeable and diverse drug data samples, include complicated quantum circuits for a more comprehensive chemical space exploration, and investigate hybrid models for multi-class drug classification, combination therapy prediction, as well as real-time clinical decision support to utilize quantum advantages to expedite drug discovery and treatment processes.

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