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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