

Womanium Global Quantum Open Project Proposal Quantum Drug Discovery

Drug discovery is the process of identifying chemical entities that are good therapeutic targets. My proposal outlines using Quantum Machine Learning to find Acetylcholinesterase (AChE) inhibitors as targets in Alzheimer's disease (AD). Machine Learning and AI help find the most feasible targets in the least amount of time, leading to cost benefits for pharmaceuticals through the clinical trial phase.

AD is the most common form of dementia causing cognitive disabilities for millions of people around the world. AChE inhibitors are a common treatment for AD, examples of drugs include donepezil, galantamine, and rivastigmine. These drugs compensate for the death of cholinergic neurons and offer symptomatic relief.

The project characteristics are the following.

1. The main idea is to develop a hybrid quantum machine learning algorithm as a starting step followed by exploring the higher dimensional Hilbert space using a pure Quantum Machine learning algorithm to classify whether the drug can be an active or inactive element to the target protein.
2. The project initially focuses on minimizing the impact of Alzheimer's disease and becomes a more generic framework for any disease in the later stages.
3. We will be initially focussing on Acetylcholinesterase enzyme as the drug target for Alzheimer's disease. The model allows you to predict the bioactivity towards inhibiting this enzyme.
4. We will be using Open Source dataset of various drugs and their bioactivity on various targets to train the Quantum Machine learning model.
5. The model loss is characterized by a Cross Entropy Loss metric. Since we have only 2 classes we can use Binary Cross Entropy Loss.
6. The accuracy of the model is determined directly by just finding the number of correct predictions divided by the total number of samples.
7. With this trained model, we can test whether any new drug samples from the test can have an action to this enzyme using a Web Based Interface.

Through this open source project, technologists can learn about bioinformatics, classical Machine learning techniques, Data cleaning and handling, Quantum Computing and Quantum Machine learning. The project also enables people to test the performance model in real quantum devices in presence of noise.

I appreciate any feedback and suggestions for the drug discovery framework development. Feel free to contact me for any questions.