ProteinQure

Our company, ProteinQure, will use quantum computing and artificial intelligence for the computational design of protein-based drugs. These drugs are hard to design because we only have structural data for 150,000 proteins. However, in small peptides alone there are 10^{65} potential amino acid sequences. Reinforcement learning and molecular dynamics simulations are the key to exploring the vast therapeutic potential of this space. We are computationally performing lead generation and optimization of drugs using this novel approach (**Fig. 1**)

Quantum computers speed up the molecular dynamics simulations. We are performing computational optimizations required to simulate protein folding (**Fig. 2**) with quantum computers and using these outputs in our classical algorithms. This speed up increases our iteration speed so that we can perform reinforcement learning on the candidate amino acid sequences. PQ.zero will enable the iterative refinement of protein-drugs for binding affinity, stability, or immunogencity, with an initial focus on cyclic peptides.

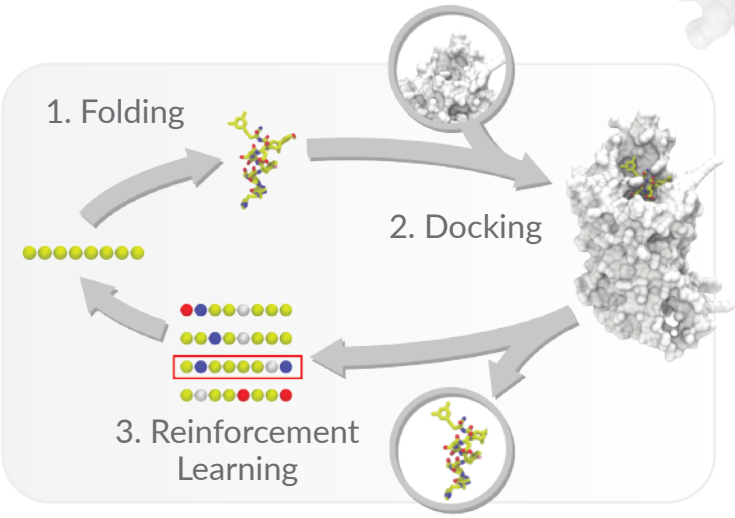

Fig. 1 ProteinQure protein design engine (PQ.zero). Utilizes successive folding, docking, and mutation to optimize binding to a target linked with disease (glucagon receptor shown).

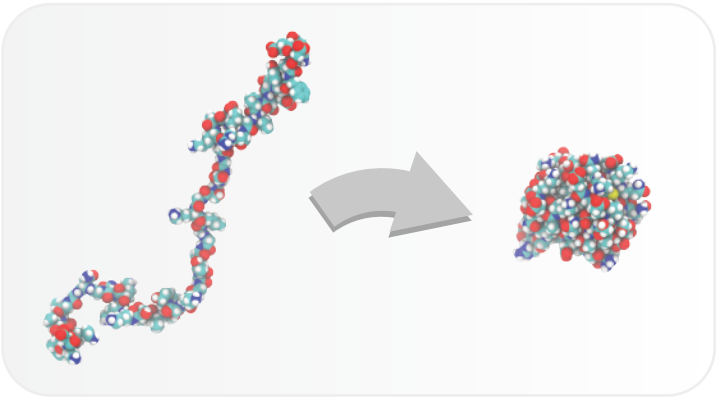

Fig. 2 Representation of the protein folding process.

ProteinQure is a top participant in University of Toronto's world class incubator - the Creative Destruction Lab. The company has received funding and access to quantum computers in the Quantum Machine Learning stream.

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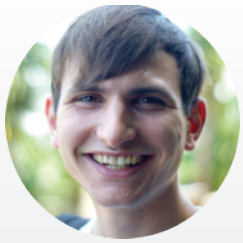

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