

Quantum-Aided Drug Design for Inhibiting Protein-Protein Interactions for Emerging Threats

DARPA Imagining Practical Applications for a Quantum Tomorrow (IMPAQT) Final Report



Introduction

The DARPA IMPAQT ARC Opportunity solicited ideas to explore the following question: What are the applications for a quantum system with $N^*q > 10,000$ as a co-processor for a classical computational system?

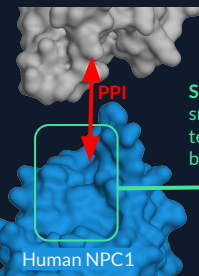
DARPA contracted PolarisQB to expand our Quantum-Aided Drug Design (QuADD) for inhibiting protein-protein interactions (PPIs) for emerging threats.

Advances

- Quantum utility: QAOA continually discovers unique optimal molecules at a steady rate while the classical sampler struggles to find new molecules
- Links to details on [Sextant](#) and our [hybrid quantum QAOA sampler](#)
- To learn about our wet lab results for small molecules generated with quantum computers, [contact us](#).

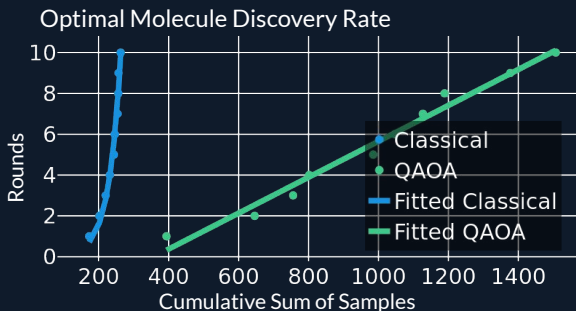
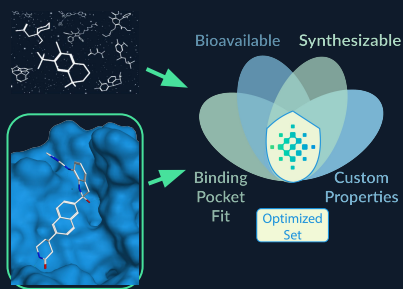
Input: 3D coordinates of the PPI interface

Ebola Virus Protein



Sextant: Builds small molecule templates into binding pocket

QuADD: The quantum computer uses the template and binding pocket and searches a massive chemical space of fragments to identify top candidates



Comparison to Classical solutions: In the pursuit of optimal molecules, the QAOA approach consistently uncovers new molecules, where classical methods, like Simulated Annealing, face challenges in sustaining the discovery of novel candidates.

Output: Library of 470 lead-like small molecules in 3D conformations in the protein pocket

