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

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

PolarisQB

Introduction

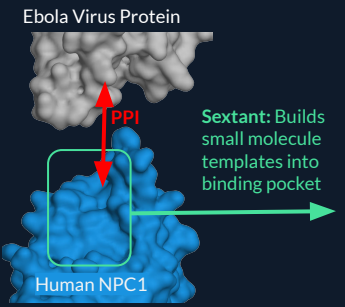
The DARPA IMPAQT ARC Opportunity solicited ideas to explore the following question: What are the applications for a quantum system with N*q > 10,000 as a co-processor for a classical computational system?

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

Advances

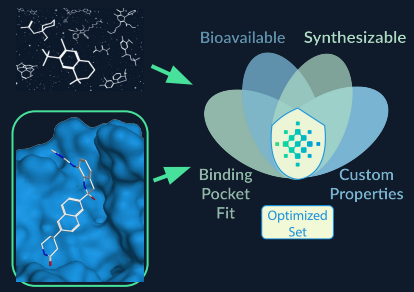
- Quantum utility: QAOA continually discovers unique optimal molecules at a steady rate while the classical sampler struggles to find new molecules
- Links to details on Sextant and our hybrid quantum QAOA sampler
- To learn about our wet lab results for small molecules generated with quantum computers,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

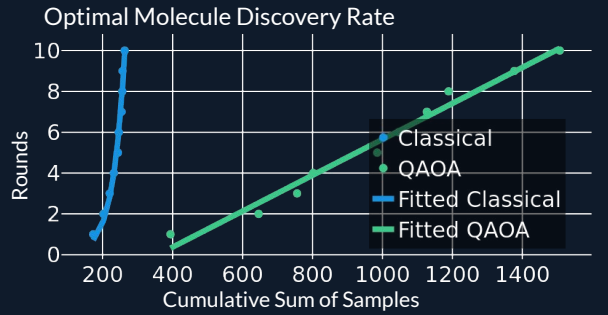
Input: 3D coordinates of the PPI interface



Sextant: Builds small molecule templates into binding pocket

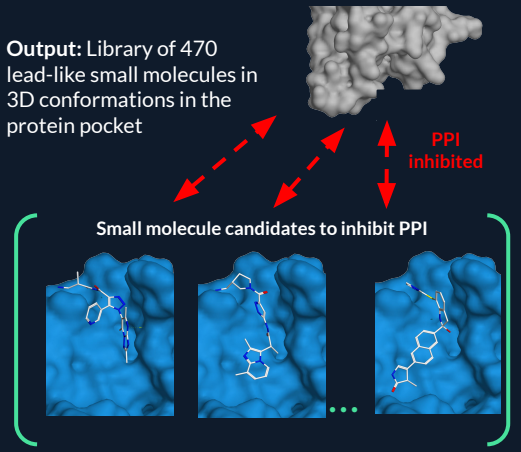
QuADD: The quantum computer uses the template and binding pocket and searches a massive chemical space of fragments to identify top candidates





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



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