POLARISqb Receives DARPA IMPAQT Funding to Advance Quantum Computing for Drug Design

The Defense Advanced Research Project Agency (DARPA) awarded POLARISqb a research contract in support of their work designing drugs with quantum computers. The contract is a part of the Advanced Research Concept topic Imagining Practical Applications for a Quantum Tomorrow (IMPAQT). POLARISqb has been developing quantum computing methods for drug discovery since their inception in 2020. Since then, they successfully built the first drug discovery pipeline that uses a quantum computer and released the first ever quantum computing powered SaaS for drug discovery, Quantum-Aided Drug Design (QuADD). With this DARPA contract, POLARISqb will expand their methods and translate them to work on different quantum computing architectures, allowing them to take advantage of predicted quantum advancements in the coming years.

The DARPA-funded project is "Quantum Computing Solutions for Inhibiting Protein-Protein Interactions for Emerging Threats." The objective is to make a novel variational quantum algorithm (VQA) that identifies small molecules that inhibit protein-protein interactions (PPIs), one of the most challenging areas of drug design. Many emerging threats, such as the Ebola virus, and constant threats, such as cancer, are caused by PPIs. Modulation of PPIs is a complicated area of drug design because the targeted interface is large, driven by hydrophobic interactions, flat, and without features. As a result, it is difficult to identify small molecules that are large enough to block a PPI while also being small enough to be bioavailable. The novel VQA will identify these "hard to find" molecules from a vast solution space that is accessible only with quantum-computing methods.

DARPA has been deeply involved in the development of quantum hardware and quantum platform technologies. As quantum computing advances, it has the potential to fundamentally change the way we solve computationally-complex problems. This IMPAQT award will allow POLARISqb to explore solving novel approaches to existing chemistry problems that would take too long or cost too much to solve on classical hardware. Dr. Anna Petroff, the computational chemist for the project, is leading the modeling of biochemical features of PPIs. Maurice Benson, Principal Investigator on the project, leading algorithm development, recently said "Everyone at POLARISqb is thrilled and honored to work with DARPA. Leveraging quantum computing has the potential to advance drug design and ultimately lead to better therapeutics"

POLARISqb translates the chemistry of drug design into a form that a quantum computer can solve. Starting with a protein binding pocket that is associated with a disease state, POLARISqb's programs search a chemical space of 1030 molecules for preclinical drug leads that are bioavailable, synthesizable, and complement the binding pocket. By searching a space that is many orders of magnitude greater than what conventional methods can access, the resulting set of molecules is more diverse and less biased. The broader industry, which relies on conventional computing and iterative wet lab efforts, takes more than three years to accomplish what POLARISqb can do in days on the QC-leveraged platform. This work has been described in Ars Technica, Nature's Biopharma Dealmakers, and Quantum Insider. For details, white papers are available here. The DARPA contract will support POLARISqb's work expanding these methods to include PPIs.