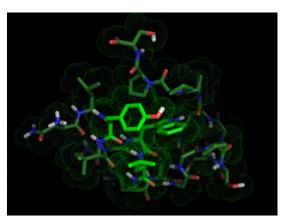


How Menten Al is Reimagining Biology with Quantum-Powered Protein Design

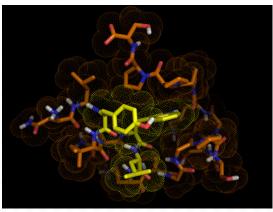
A Case Story

I'm using the D-Wave quantum annealer to solve the protein sequence design problem.
One application is the rational design of new drugs able to target antibiotic resistance mechanisms, which we hope will one day give rise to new tools to use in the clinic to fight the growing threat of antibiotic-resistant infection.

Vikram Mulligan Co-Founder - Menten Al



Trp cage mini-protein (PDB ID 1L2Y)
This simple 3-residue packing problem has 28 solutions



Solution found by D-Wave
Of the 28 possible solutions, this is optimal

Astronomically Large Search Problems

Designing or modifying proteins has wide application in drug design, materials design, and enzyme design for low-energy manufacturing. In recent years, computational protein design (CPD) techniques for molecular simulation have been used to predict sequences with new and improved functions. However, CPD involves astronomically large search problems, rapidly exceeding the capabilities of even the largest supercomputers. Using a classical-quantum hybrid approach on a D-Wave system, Menten achieved better solutions, faster, compared to a classical computer.

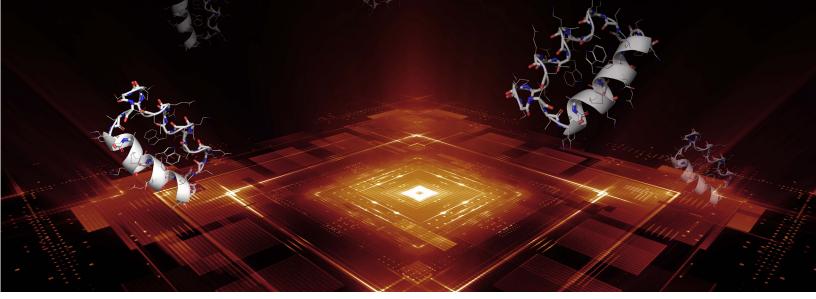
The Power of Nature Meets the Power of Quantum Computing

Combining the power of nature with the power of quantum computing is an exciting new approach for such scientific inquiry. Companies like Menten AI are harnessing the unique capabilities of quantum computers for applications in life science and biotechnology.

Menten uses cutting-edge machine learning and quantum computing to design and engineer proteins for applications in the pharmaceutical and chemical industries. Designer proteins of this sort could one day be useful as therapeutics: they could be engineered to allow patients to see better results with smaller doses of medication, as well as fewer side effects. They could also be engineered to accelerate and reduce the energy required to carry out chemical reactions important for industrial manufacturing.

Currently, protein design is a trial-and-error process, relying on undirected, evolutionary experiments and blind screening of random mutations. Menten has taken the first steps towards transforming this nebulous, non-linear process into a more rational engineering operation. By extending the capabilities of Rosetta—one of the leading software packages for protein design and structure prediction—and allowing it to interface with a D-Wave quantum processor, researchers were able to leveraging quantum annealing for the protein design problem.



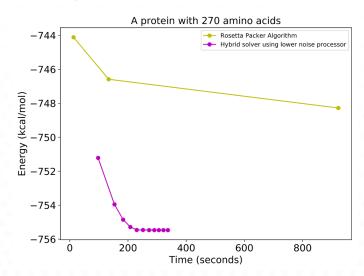


Their initial experiment—aimed at determining whether or not a quantum computer could handle the protein design problem without it needing to be simplified or reduced in size—was a success, and led to the development of the first quantum-designed molecule. As a result, Menten is now doing real, wet-lab experiments informed by those predictions.

As the research team wrote in a <u>paper</u> (submitted for initial review), "The rotamer optimization problem — the central problem that must be solved when designing a protein — maps well to the D-Wave quantum annealer without simplifying the design task or sacrificing accuracy."

The Value of Hybrid Computing

By taking a hybrid quantum-classical computing approach using D-Wave's 2000Q quantum system, Menten hopes to be able to significantly reduce the cost and time required to engineer proteins for drug design, as well as overcome the scalability challenges that limit classical approaches. The hybrid approach has already resulted in better solutions, faster:



As larger quantum computers are introduced, Menten anticipates they'll be able to tackle larger design tasks than will ever be possible on classical hardware. The efforts of Menten and others in the biomedical space will have profound implications for drug development, targeted disease therapeutics, and more.



D-Wave is the leader in the development and delivery of quantum computing systems, software, and services.

Our mission is to unlock the power of quantum computing by delivering customer value with practical quantum applications for problems as diverse as logistics, artificial intelligence, materials sciences, drug discovery, cybersecurity, fault detection and financial modeling. Learn more at www.dwavesys.com



Jumpstart your quantum application development through Leap, D-Wave's quantum cloud service. Leap provides:

- Live access to D-Wave quantum systems
- Quantum-classical hybrid solvers you can simply submit your hard problems to
- Open-source software and a comprehensive online IDE for developing your own quantum applications
- Interactive demos, code examples, documentation, and a vibrant online community

Designed for developers, researchers, and forwardthinking enterprises, Leap speeds the development of real-world applications.

Sign up today at cloud.dwavesys.com/leap/signup/.