Menten AI is Reimagining Biology with Quantum-Powered Protein Design

CASE STORY

The Power of Nature Meets the Power of Quantum Computing

By taking a hybrid quantum-classical computing approach using D-Wave's Advantage system, companies like Menten AI are harnessing the unique capabilities of quantum computers for applications in life science and biotechnology.

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.

in 2020, Menten announced the development of the first successful process using hybrid quantum programs to determine protein structure for de novo protein. According to Menten CEO Hans Melo, the results have been extremely encouraging, with the hybrid quantum approach often outperforming classical solvers. Menten AI's unique protein designs have been computationally validated, chemically synthesized, and are being advanced to live-virus testing against COVID-19.

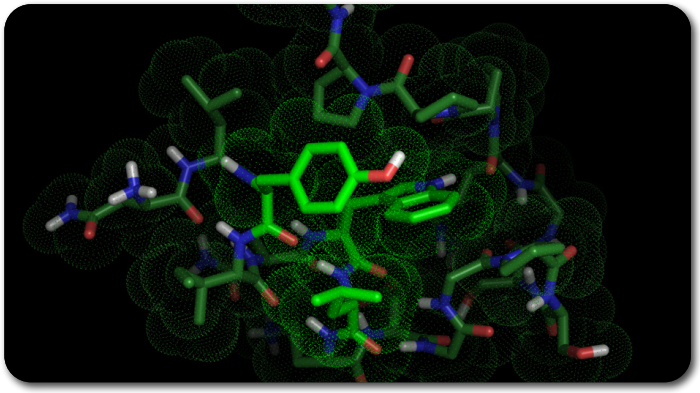
Astronomically Large Search Problems

Designing or modifying proteins in this way has wide applications 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.

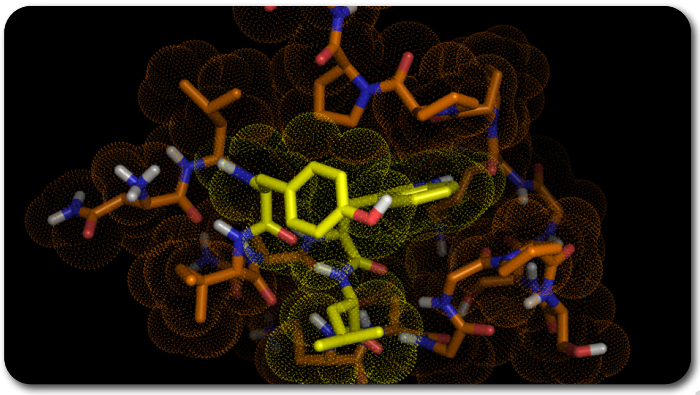
As the research team wrote in a recent paper (submitted for initial review), *"The rotamer optimization problem — the central problem that must be solved when designing a protein — maps well to the D-Wave quantum annealer without simplifying the design task or sacrificing accuracy."*

"Using hybrid quantum applications, we're able to solve astronomical protein design problems. We've seen extremely encouraging results, with hybrid quantum procedures often finding better solutions than competing classical solvers for de novo protein design. This means we can create better proteins and ultimately enable new drug discoveries."

Hans Melo
CEO & Co-Founder - Menten AI



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

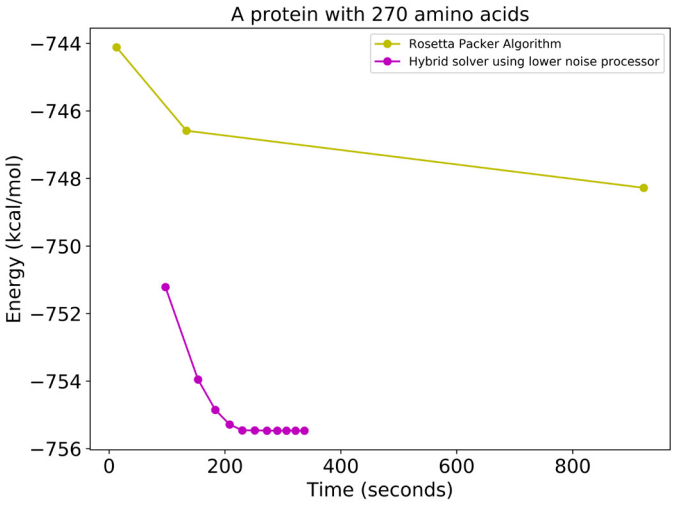


Solution found by D-Wave
Of the 28 possible solutions, this is optimal

The Value of Hybrid Computing

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.

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 leverage quantum annealing for the protein design problem.



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.

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.