Menten AI Battles COVID-19 with Quantum Peptide Therapeutics

CASE STORY

To Boldly Go Where No One (nor Nature) Has Gone Before

When researchers at Menten AI think about proteins, they're not trying to figure out how to pack another serving into your daily energy shake. Instead, they're thinking about the molecular building blocks of life. These chains of amino acids are how nature performs chemistry; they enable every dynamic function that takes place inside our bodies and the bodies of all other living things.

Over the last few years, there has been a rapidly growing interest among scientists in developing new proteins which can facilitate therapeutic processes and power new drugs, replace toxic chemicals and enzymes currently used in industrial applications, and more. This is easier said than done. Until recently, protein design research had been an expensive, lengthy, and suboptimal process of trial and error, relying on undirected evolutionary experiments and blind screening of random mutations.

Advances in computing technology have allowed companies like Menten to begin transforming the protein design process into a more rational engineering operation, but this has revealed new challenges. For one thing, there is a limit to how much of the potential protein landscape even the most powerful supercomputers can explore. For another, while researchers are now able to experiment with directed evolution—taking naturally occurring proteins and mutating them in purposeful ways—this only works as long as you already know what your starting point is. For most possible proteins, a natural starting point doesn't exist.

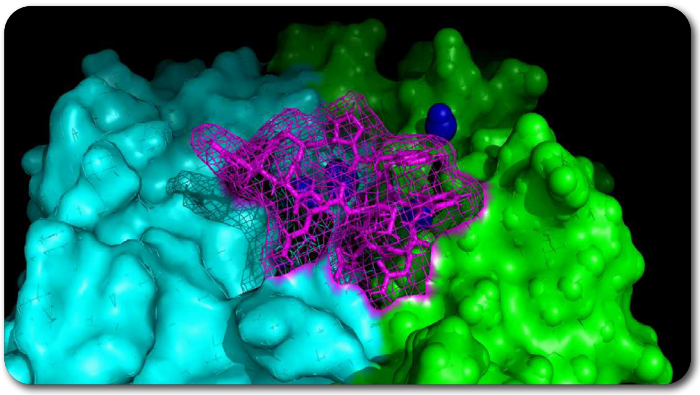
"How do we explore a space that nature—even after four billion years—hasn't had a chance to explore?"

asked Hans Melo, Menten CEO.

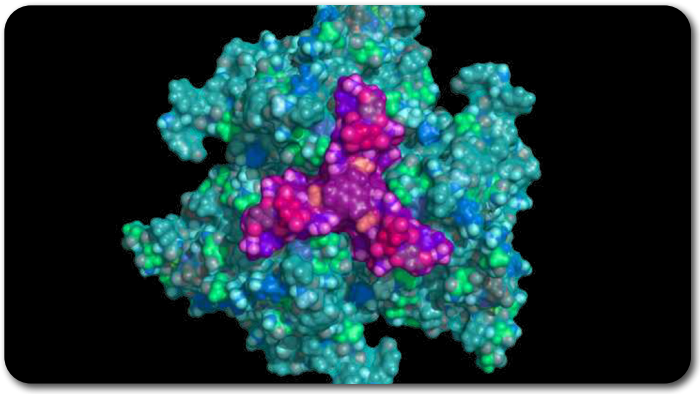
The answer: the power of quantum computing.

"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



Protein with a peptide 'backbone' or scaffold in place



Designed SARS-COV-2 inhibitor peptide

Menten's first step towards revolutionizing protein design was simple: to determine whether protein design problems could be mapped onto quantum computers without needing to simplify them or reduce their size. 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 successfully leveraged quantum annealing to generate protein designs at scale without sacrificing accuracy.

Further experiments focused on the viability and energy cost of the proposed solutions in a lab setting. By using a hybrid quantum-classical approach, the Menten team was able to explore an even larger piece of the protein landscape and head off failures later in the process.

Harnessing Quantum Peptide Therapeutics to Battle COVID-19

With the rise of COVID-19, Menten set its sights on using quantum computing to explore options for creating antiviral binders to fight the disease.

Peptides are small chains of amino acids which can be used as they are or combined with other peptides to form proteins. Designing them is a bit like creating a puzzle piece. For purposes of drug design, researchers need to be able to identify the specific protein they want a drug to be able to target and what properties the peptide they're building will need to have in order to do that. This requires the ability to move individual atoms to specific positions so that the molecule will bind to the protein securely and have the desired effect.

The SARS-CoV-2 spike glycoprotein—the protrusion which interacts with the receptors on our cells and allows COVID-19 to infect them—can be in one of two positions or modes at any given time: open and closed. In order to infect healthy cells, it must move from closed to open, a bit like turning the knob on a faucet so the water can begin to flow. Stopping the process which allows these glycoproteins to open would prevent them from attaching to our cell receptors.

With this goal in mind, Menten created a fixed 'backbone' to serve as a starting point for the peptide. Through D-Wave's hybrid solver, they used the D-Wave Advantage™ quantum computer to explore a huge combinatorial space and determine the optimal composition and configuration of the side chains or branches. The challenge was to design the peptide in such a way that it binds as closely, specifically, and seamlessly as possible to its target. This maximizes effectiveness while reducing the odds of the peptide attaching itself to anything besides the target, which could cause complications or side effects.

Using D-Wave's hybrid solver, Menten produced several different peptide designs. Two key features of these peptides are that they are designed from scratch (in de novo or "from the new") and made with both natural and non-natural amino acids. These new molecules are an expansion of the fundamental building blocks of life beyond those that have been used by nature up until now. The designs have been computationally validated and chemically synthesized and are currently being used in live-virus testing. Initial results are anticipated to be announced in the near future.