Quantum in Life Sciences: The Future is Now

Drug discovery is a high-risk, high-reward field, where a blockbuster therapy can deliver life-changing clinical benefits to millions of patients and generate billions of dollars in profit. But the road to regulatory approval is littered with innumerable failed programs, and more than 90% of new drug development efforts ultimately prove fruitless.[1]

Quantum computing could help pharma and biotech companies to stack the odds in their favor, and the industry is taking notice of this promising new technology. In a survey from last summer[2], 82% of life science organizations agreed that quantum computing will have a commercial impact within the next decade—and nearly a third stated that they would begin evaluating such systems within the coming year.

Computer-aided drug design is already a mainstay of the pharmaceutical industry, and the adoption of quantum computing could enable faster and more efficient identification of molecules with promising biochemical and therapeutic properties. But quantum computing could also contribute to other scientific and operational aspects of the life sciences industry as well, offering businesses a way to replace inefficient trial-and-error processes with an automated, engineering-based approach.

Quantum Use-Cases in Life Sciences

The drug discovery process involves several areas that are well-suited to hybrid-quantum computers, which optimize the combined use of both classical and quantum computing resources. Quantum computers, and especially quantum annealing systems like D-Wave's, are well-suited to deliver optimal solutions to combinatorial optimization problems with large numbers of variables and constraints.

These powerful computing capabilities can potentially be leveraged to tackle thorny problems at many stages of the drug development process. This could include crunching 'big data' from clinical studies to guide precision medicine efforts for various diseases, or identifying and optimizing chemical compounds with promising therapeutic properties.

Here are a few examples of applications in the life sciences that could benefit from the application of quantum resources in the coming years:

- **Lead generation for small-molecule drugs:** How can you accelerate the identification of chemical compounds that selectively bind a disease-related protein target with minimal off-target effects?
- **Protein structure prediction:** How can you accurately determine the three-dimensional structure of a protein of interest based only on its amino acid sequence?
- **Protein engineering and design:** How can you generate novel, complex biomolecules that selectively activate, inhibit, or otherwise modulate important biological functions?
- **Precision medicine:** How can you find the hidden patterns in your clinical datasets that might reveal actionable connections between specific genetic features and human disease?
- **Pathology and imaging analysis:** Can you discriminate subtle features in patient CT, MRI, X-ray, or histology images that might produce a more accurate diagnosis or enable more reliable disease monitoring?
- **Manufacturing and logistics:** How can you optimize the management of your reagent supply chain to maximize the stability and cost-effectiveness of your production processes?
- **Clinical Trials:** How can you streamline, standardize, and de-risk clinical trials to reduce costs, accelerate development, and increase the likelihood of success?

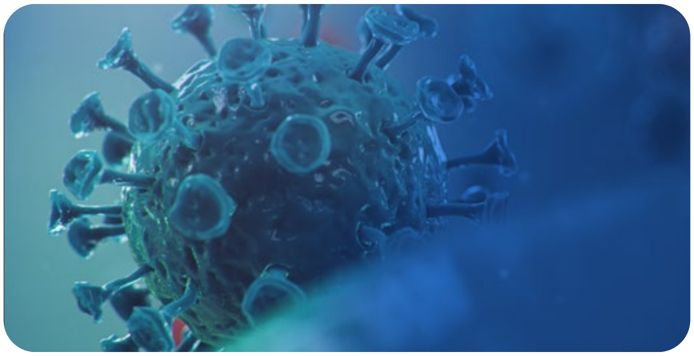
Quantum Use-Case Spotlight: Protein Design

We're using the D-Wave quantum annealer to solve the protein sequence design problem.

—Vikram Mulligan Co-Founder, Menten AI

Menten AI routinely makes use of D-Wave quantum computing to assist in the design of novel therapeutic peptides—short strings of amino acids that can act as potent drugs. With the rise of COVID-19, Menten set its sights on using its quantum annealer-powered approach to explore the development of antiviral peptides that might block infection by the SARS-CoV-2 virus.

SARS-CoV-2 relies on the spike protein molecules that stud its surface to bind certain protein receptors expressed by cells in our airways. This in turn allows the virus to infiltrate the cell and produce more viral particles.



For successful infection to occur, the viral spike protein must transition from a 'closed' structure to an 'open' structure, which exposes protein features that can recognize and bind cellular receptors.

With this mechanism in mind, Menten set about designing a peptide that could thwart infection by trapping viral spike proteins in their closed state. Their researchers first created a fixed chemical 'backbone' as a scaffold for the peptide, and then used the D-Wave Advantage™ system to explore the huge combinatorial space of possible amino acid compositions for that scaffold. This quantum-assisted search made it possible to identify molecules that might be especially well-suited for binding and inhibiting the spike protein.

D-Wave's hybrid solver enabled the Menten team to produce several promising peptide designs. Critically, these different molecules were all developed from scratch – without using a known protein as a starting point – and make use of a combination of both naturally-occurring and synthetic amino acids. These designs have been computationally validated and chemically synthesized, and are now being tested for their ability to trap the SARS-CoV-2 spike protein in its closed, inactive state.

1. https://www.nature.com/articles/d41573-019-00074-z
2. https://www.sri.com/press-release/almost-one-third-of-life-science-companies-set-to-begin-quantum-computing-evaluation-this-year