BroadBranch Advisors

# Quantum Computing in Drug Discovery

**Advances in computing catalyzed a shift from analog to digital electronic processing, and now the computing industry is at the precipice of a new more powerful frontier driven by the development of quantum computing.**

Quantum computing is a shift in how data is processed that enables faster calculation speeds utilizing a different set of physical properties compared to digital computing. The benefits of increased speed and processing complexity have implications across industries (finance, logistics, security, etc.) but will enable a new degree of potency in the life sciences, particularly drug discovery, where the next phase of understanding has largely been limited by current computational bottlenecks.

## HARNESSING QUANTUM COMPUTING TO REVOLUTIONIZE DRUG DISCOVERY

The core of quantum computing's processing power comes from the qubit – compound word built from 'quantum' and 'bit' terminology used in traditional computing. Digital computing bits utilize binary states (0s or 1s) to generate logic systems, whereas a 'qubit' can exist in any number of states ***between*** 0 and 1. This increased complexity of quantum computing's fundamental processing unit enables the execution of complex logic systems in a fraction of the time a digital computer requires.

Given the current pace of advances in quantum computing the industry expects to have the technology ready for commercialization by 2030, with full consumer accessibility shortly thereafter impacting industries globally. Within drug discovery, for example, quantum computing's greatest impact will primarily be in the research and development phase where advanced computing power is expected to be able to allow researchers to characterize molecular states and their target interactions at the sub-atomic level.

Currently, computer-assisted drug discovery (CADD) is the major *in silico* methodology used in early drug discovery. While traditional computing faces challenges when simulating large, complex biomolecular systems, particularly at the sub-atomic level, quantum computing offers a more efficient paradigm for simulating these systems, providing a more authentic representation of intermolecular interactions.

## INTERTWINING A LANDSCAPE OF COMPUTING AND DRUG DISCOVERY PLAYERS

Various large computing players such as IBM and Amazon are leading the quantum computing hardware and accessibility charge for drug discovery applications. Today IBM provides access to quantum-based compute capabilities via a cloud-based platform. A collaboration between IBM and Algorithmiq pressure tested IBM's capabilities in conjunction with Algorithmiq's drug discovery platform to demonstrate the improved capabilities of quantum computing over digital


computing in early drug discovery applications. Algorithmiq's techniques showed reduced runtime and error mitigation yielding improved speed and accuracy over classical algorithms, but drug discovery applications are anticipated to take further compute power for full realization than are currently available. Although offering fewer quantum capabilities with fewer qubits than industry leader IBM, Amazon Web Services (AWS) offers public, cloud-based access to quantum processing and hardware that could be leveraged to run platforms and quantum algorithms for drug discovery customers.

Other companies are focusing on the development of quantum algorithms and platforms to support drug discovery. Atos, a quantum machine learning company, develops quantum algorithms to accelerate modeling, simulation and optimization of targets. Atos has collaborated with IBM to offer end-to-end quantum computing capabilities. Menten AI focuses on developing an advanced generative AI platform for the purposes of designing and optimizing peptides for



therapeutics. Menten AI has collaborated with Xanadu at the software level and D-wave System's computing capabilities during the development of their platform. Accenture has used quantum computing platforms for early drug discovery and established a collaboration with Biogen to demonstrate the potential to improve the overall drug discovery process when employing quantum computing.

## READYING FOR A QUANTUM COMPUTING TRANSITION

The integration of quantum computing holds a great deal of potential across the drug discovery workflow. Players providing quantum computing capabilities, leveraging quantum computing for their algorithms and platforms in their discovery process, or developing and optimizing the technology to better serve customer needs should recognize the wide range of involvement opportunities accompanying this inevitable shift in the landscape. Regardless of where companies choose to establish their stake in the market, a plan of action for the digital to quantum transition will be necessary for success. The promise of speed and capability quantum computing offers will put companies waiting to "catch up" to their competitors that have already adopted quantum computing at a severe disadvantage.


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