WILL QUANTUM COMPUTING TRANSFORM BIOPHARMA R&D?

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Of the many industries in which quantum computing is expected to have a far-reaching impact, biopharma is among the most promising. Quantum computing has the potential to significantly accelerate, enhance the quality of, and reduce the costs of data-rich R&D processes. The earliest uses are likely to involve the early stages of R&D (drug discovery and design), but the impact will extend into the later stages of R&D, thanks to higher clinical success rates from better early design.

Quantum computing is still very much an emerging technology, and the pathway to practical application remains under construction. However, the technology is graduating from the lab and heading for the marketplace. Google announced that it had achieved "quantum supremacy" in October 2019, IBM has committed to doubling the power of its quantum computers every year, and numerous other companies and academic institutions are investing billions toward making quantum computing a commercial reality. Biopharma companies have the potential to benefit significantly from this technology—and those that begin taking the right steps now may gain a lasting advantage.

As with any emerging technology, much of the potential value lies in how commercial enterprises apply new capabilities to improve core processes. We believe that quantum computing is very likely to transform the early stages of pharmaceutical R&D over the coming decades—and that it will provide near-term benefits as the technology matures. But its actual impact will depend in large part on how biopharma companies learn to use it. Aside from quantum computing hardware and software, keys to success will include talent, new ways of working, and partnerships. Early movers will almost certainly gain advantages that followers will have a tough time matching.

Current Challenges in Pharmaceutical R&D

The biopharma R&D process—from drug discovery to development—is a costly,

lengthy, and risky endeavor. A new drug typically takes 10 to 15 years to progress from discovery to launch, and the capitalized costs exceed $2 billion. The success rate is less than 10% from entry into clinical development to launch. For these reasons, biopharma companies count on a few blockbuster drugs to realize payback of the more than $180 billion that the industry spends each year on R&D.

Computational tools are already key components of drug discovery and development. In many instances, they have significantly shortened the time companies spend on drug optimization. Researchers rely on high-performance computing—using powerful supercomputers or massive parallel processing—to perform in silico modeling of molecular structures, mapping of the interactions between a drug and its target, and simulations of the drug's metabolism, distribution, and interactions in the wider human system.

For example, computational chemistry algorithms aim to predict how a potential drug molecule will bind to specific target proteins, by modeling the binding energy of interaction. Because many of these algorithms do not scale well with the number of atoms involved, however, they are often limited to relatively simple molecular structures. For example, IBM has estimated that fully and accurately modeling the base-state energy of the penicillin molecule, which is composed of 41 atoms, would require a classical computer with more transistors than there are atoms in the observable universe.

How Quantum Computing Can Reshape Drug Discovery

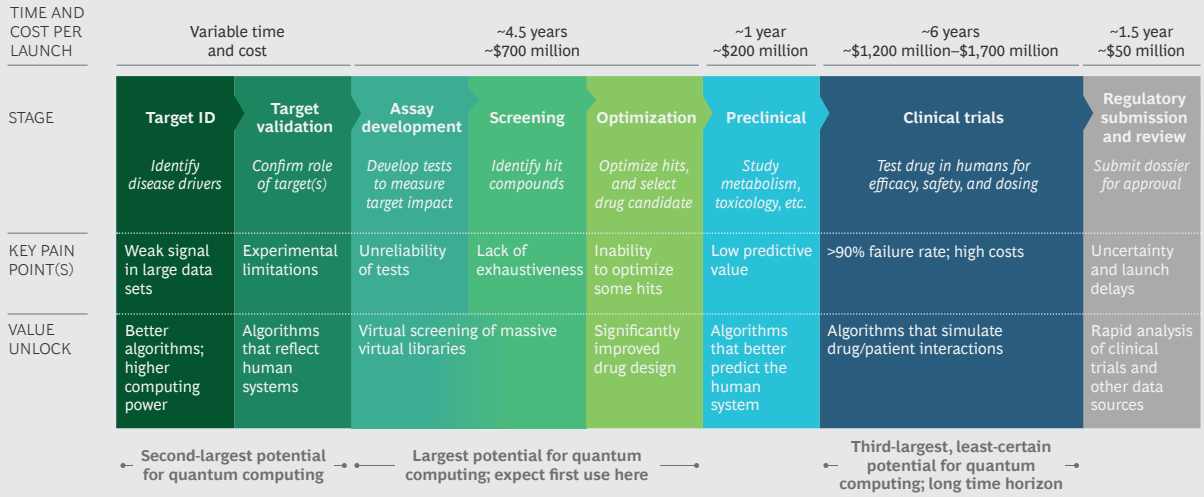
Quantum computers work fundamentally differently than classical computers, and these differences give them the power to solve certain classes of problems that classical computers cannot. Classical computers are built on bits that have values of zero or one. In contrast, a quantum computer uses quantum bits (or qubits), which can be overlays of zeros and ones (meaning part zero and part one at the same time). Rather than working in isolation, qubits become entangled and act as a group, which helps enable quantum computers to achieve an exponentially higher information density and computing speed than classical computers. This gives them an advantage over classical computers in solving four types of problems: combinatorial optimization, differential equations, linear algebra, and factorization. Whereas modeling penicillin on a classical computer would take 10^{86} bits, it could take as few as 286 qubits on a quantum computer.

Quantum computers provide powerful tools for studying complex systems such as human physiology and the impact of drugs on biological systems and in living organisms. We believe that quantum computing will have numerous uses in pharmaceutical R&D, especially in the early phases of drug discovery and development. (See Exhibit 1.)

Take optimization. Currently, the process of modifying the physio-chemical properties of hit compounds to produce lead compounds and, ultimately, drug candidates still mostly relies on expensive and time-consuming experimental methods. The biopharma industry already applies quantum mechanics for energy calculations and structural optimization, especially in molecular docking and quantitative structure-activity relationship analyses. Quantum mechanics–enabled synthetic chemistry gives researchers the tools to preclude potentially inactive compounds and to support the synthesis of more challenging compounds. As quantum-based virtual screening and optimization leverage molecular simulations, it is possible that researchers will someday be able to combine both into a single in silico workflow.

Or consider screening. Virtual screening tools tend to be cheaper and faster than chemical processes for screening large compound libraries against a target of interest. But the usefulness of virtual tools depends on their ability to accurately predict hits, especially for complex molecules. Quantum computing has the potential to transform virtual screening through physically precise modeling of drug-target inter-

Exhibit 1 | The Potential Impact of Quantum Computing on the Drug Discovery and Development Process



Sources: Paul et al., "How to improve R&D productivity: The pharmaceutical industry's grand challenge," *Nature Reviews Drug Discovery* 9(3):203–214 (2010); BCG experience and analysis.

actions and efficient screening of massive virtual libraries. Another complication is that building a tool to test compounds for the desired impact on a target during screening is a slow, labor-intensive lab process. By improving in silico screening and compound validation, quantum computing could reduce the need for costly and time-consuming in vitro testing. Eventually, quantum computing could permit end-to-end in silico drug discovery.

Quantum computing may also be useful in the target identification phase by enabling deeper exploration of complex multifactorial diseases that require the modulation of multiple targets. In addition, there could be applications in clinical development.

The possibility of step changes in predictive capability is not a distant dream. Hybrid quantum-classical approaches that can predict molecule structure should be available within the next five years, allowing more-effective structure-based drug design of small molecules. A number of startups are developing virtual screening tools that use 3D representations of molecules derived from quantum mechanics to determine interactions between drugs and their targets.

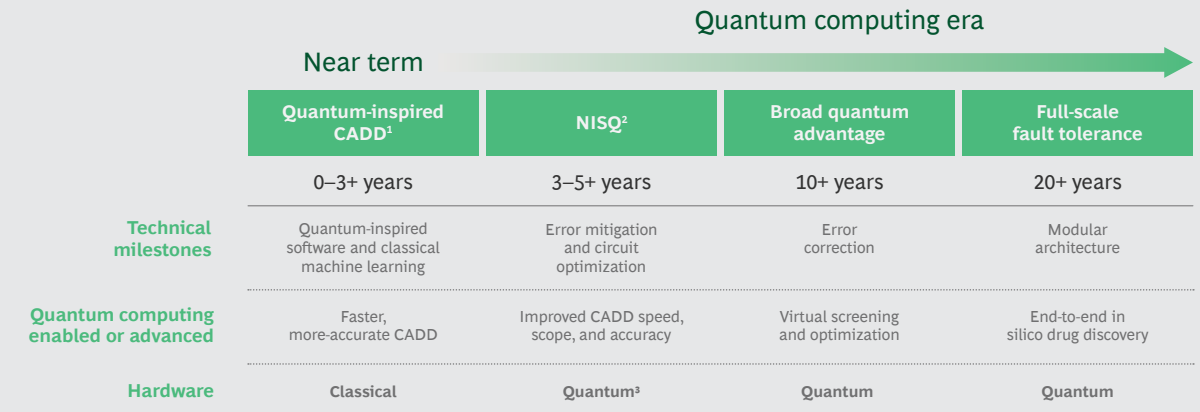
How Biopharma Can Get Ready for Quantum Advantage

While the long-term promise of quantum computers may be transformative, the machines available today have serious shortcomings related to capacity, stability, and reliability. These issues must be overcome before companies can put quantum computers into practical service. We expect this journey to develop through four distinct phases, during each of which capabilities, applications, and business income will steadily increase over time. (See Exhibit 2.)

The earliest uses involve the computer-aided drug discovery (CADD) applications described above. The next decade will be defined by so-called noisy intermediate-scale quantum (NISQ) devices, which increasingly will be able to perform useful, discrete functions, but will also be plagued by high error rates that limit their functionality. In three to five years, error mitigation techniques, along with better hardware and algorithms, should begin to support useful business applications.

Error-corrected machines will achieve true quantum advantage, outperforming classical computers in time, cost, or quality for the applications we have outlined. But er-

EXHIBIT 2 | The Journey Toward Quantum Drug Discovery



Source: BCG experience and analysis.
[1]CADD = computer-aided drug discovery.
[2]NISC = noisy intermediate-scale quantum.

ror correction is still at least a decade away. The next milestone after that is full-scale fault tolerance, at which point quantum computers could enable full in silico drug discovery and design.

Harnessing technology during the NISQ decade requires mastery of four areas: quantum hardware- and software-based solutions, talent, new ways of working, and partnerships.

Quantum Hardware- and Software-Based Solutions. In addition to the hardware advances that large end-to-end providers such as Google, IBM, and Honeywell are pursuing, emerging companies such as D-Wave, Rigetti, and Xanadu are active. As happened in the early days of the semiconductor industry, quantum computing hardware manufacturers are aiming to develop circuits optimized to solve particular problems, such as molecular docking.

For example, IBM is taking this approach to produce specialized circuits for "hidden shift" and quantum Fourier transform algorithms. "When it comes to near-term applications, the beautiful work will happen at the cross-section of business needs and quantum circuitry so that the circuit itself determines the application," IBM's head of quantum computing, Jay Gambetta, told us.

Because they work differently from classical computers, quantum computers require new software and algorithms. Specialists such as ProteinQure, GTN, Rahko, Menten AI, and Qulab are pioneering quantum drug-discovery algorithms. By partnering with these and larger companies, biopharma companies may be able to shape optimized circuit-to-application solutions and realize value more quickly.

In the meantime, the massive classical computing industry continues to deliver performance improvements (through supercomputers, HPC, and GPUs) and better algorithms that will help bring value to biopharma companies even sooner. Quantum computing has introduced new ways to approach problems, inspiring new algorithms that run on classical hardware. Microsoft, which has dubbed these new techniques "quantum-inspired," has just released a quantum-inspired chemistry library with 1QBit to run on Azure Quantum. Companies such as Silicon Therapeutics, XtalPi, Qubit Pharmaceuticals, Atomwise, Turbine, and Benevolent AI are using quantum-inspired approaches, often in combination with machine learning, and aim to achieve quicker and more-accurate drug discovery. Proven quantum computing algorithms boost machine learning training, so this approach will accelerate as NISQ machines become more powerful.

Talent. How companies decide to tackle specialized software development—internally, externally, or with a combination of the two—will have major implications for their talent needs and their organizations. Companies will need skilled scientists and technicians, including hardware and software experts, to handle these tasks. Such talent is in short supply—and the supply is shorter still for jobs that require quantum computing knowledge or experience. Early movers have the opportunity to establish a skills advantage by becoming recognized centers of commercial advances in quantum computing. Companies such as Airbus already offer quantum training programs to prepare their engineers for the future.

New Ways of Working. In order to derive value from new approaches such as quantum computing, companies may need to change their processes. Building internal quantum computing capabilities requires not only relevant quantum skills but also collaboration between research scientists and pharma businesspeople, and work with talent in other technical fields such as artificial intelligence and machine learning. The new solutions promise a step change over current CADD tools in both accuracy and speed (for example, Atomwise claims a 10,000x improvement in hit rates and 100-times-faster screening times, and other players point to similar improvements) that will open up radical new ways to design drugs. But to capture the value, companies must change their processes and, potentially, their organizational structure, in addition to adopting agile ways of working. An agile approach enables faster and more efficient testing and iteration of promising therapeutic candidates and technological advances. In other industries, early leaders that have adopted agile have seen as much as a doubling of the speed of their new product development.

Partnerships. Innovation is a much more fragmented and varied endeavor today than ever before. More young companies in more places are pursuing more new avenues. One result of this fragmentation and diversity of effort is that although knowledge, skills, and information are much more accessible, they are also harder to harness because they reside in more numerous and more disparate places—geographically, industrially, and functionally. Investing in partnerships dedicated to building custom solutions that address the most crucial drug discovery challenges is an effective way to gain a foothold in the emerging quantum computing ecosystem. As BCG has observed before, deep technologies require a more thorough analysis of the stakeholders' interdependencies and more precise value creation models in order to accurately determine how to align goals, set strategies, and organize for interaction with others.

How to Get Started

Quantum computing is likely to have a profound impact on biopharma R&D, potentially changing the competitive set and dynamics of drug discovery. A quantum-advantaged world will probably witness a race to find and patent the best molecules for a given target. This in turn will set off a "landgrab" of the most promising molecules, targets, and biological or clinical mechanisms for subsequent exploration. It's also possible that tech players will enter drug discovery, competing with pharma companies. In an extreme scenario, biopharma companies risk being relegated to focusing mainly on clinical development, medical affairs, and sales.

Biopharma should take the necessary steps now to prepare for quantum computing's role in R&D. A sensible first step would be to conduct an assessment of the probable impact of quantum, featuring a workflow analysis to identify key friction points and solution mapping to determine whether these challenges fall into quantum-advantaged problem archetypes. Companies can then identify "lighthouse" use cases and build out early.

As they move forward, biopharma companies should look for early wins that will demonstrate the value of new approaches (such as a speed-up over previous, non-probabilistic algorithms) to the rest of the

organization. Quantum-inspired algorithms that emulate quantum concepts on classical hardware or specialized NISQ-era quantum circuits are good places to start.

Ultimately, quantum computing is likely to yield greater speed and efficiency in drug discovery, improvements in existing drugs, and faster development of new drugs. It should also accelerate time to market. The technology's long-term potential is vast, but quantum computing also offers biopharma companies tangible benefits in the near term. Companies that want to play need to prepare for a quantum future now.

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Acknowledgments

The authors are grateful to Heba Arshad, Amit Kumar, Anusha Narayan, Michael Ringel, and Andrew Rodriguez for their contributions to this article.