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The quantum revolution in pharma: Faster, smarter, and more precise

Quantum computing presents a multi-billion-dollar opportunity to revolutionize drug discovery, development, and delivery by enabling accurate molecular simulations and optimizing complex processes.

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The life sciences industry, especially pharmaceuticals, is experiencing declining R&D productivity due to high failure rates of drugs during development, the need for larger and more complex clinical trials, a shift toward biologics and more complex small molecules, and a focus on complex and poorly understood diseases such as Huntington's and Alzheimer's.[1] There is an urgent need for breakthrough technological solutions, including more precise modeling tools.

AI can assist by enhancing molecular simulations and data analysis. However, it faces challenges in accurately modeling the quantum-level interactions that are critical for drug development. AI can struggle to cope with the complex, dynamic nature of chemical systems and can be limited by the availability and quality of training data.[2] These constraints can prevent AI from fully addressing the intricacies of molecular interactions, leaving significant gaps in research capabilities.

A transformational leap with quantum computing

Quantum computing (QC) is poised to transform the life sciences industry; McKinsey estimates potential value creation of $200 billion to $500 billion by 2035.[3] The source of this value, and what sets it apart from earlier technologies, is QC's unique ability to perform first-principles calculations based on the fundamental laws of quantum physics.

This capability signifies a major advancement toward truly predictive, in silico research. By creating highly accurate simulations of molecular interactions from scratch, without relying on existing experimental data, QC enables researchers to computationally predict key properties such as toxicity and stability, significantly reducing the need for lengthy wet-lab experiments, and generating high-quality data that would otherwise be unavailable for training advanced AI models.

This is not just an incremental step for R&D; it is a fundamental change that could transform the entire value chain, from initial discovery to patient delivery.

Revolutionizing research and rethinking clinical trials

QC is expected to have its most profound impact in R&D because of its dependence on molecular simulations. For example, AstraZeneca has collaborated with Amazon Web Services, IonQ, and NVIDIA to demonstrate a quantum-accelerated computational chemistry workflow for a chemical reaction used in the synthesis of small-molecule drugs.[4] QC can enhance R&D in several ways:

Precision in protein simulation. Quantum computers can accurately model how proteins adopt different geometries, factoring in the crucial influence of the solvent environment. This is vital for understanding protein behavior and identifying drug targets, and it is especially helpful for orphan proteins, where limited data hampers AI models.

Enhanced electronic structure simulations. Understanding the electronic structure of molecules is key to predicting their interactions. QC offers a level of detail far beyond that of classical methods. For instance, Boehringer Ingelheim has collaborated with PsiQuantum to explore methods for calculating the electronic structures of metalloenzymes, which are critical for drug metabolism.[5]

Improved docking and structure–activity relationship analysis. QC can provide more reliable predictions of how strongly a drug molecule will bind to its target protein, offering deeper insights into the relationship between a molecule's structure and its biological activity. This enhanced precision helps identify promising drug candidates more efficiently.

[1] John Q. Trojanowski et al., "A model for improving the treatment and care of Alzheimer's disease patients through interdisciplinary research," *Alzheimer's & Dementia*, November 2012, Volume 8, Number 6.
[2] Jian Jiang et al., "A review of machine learning methods for imbalanced data challenges in chemistry," *Chemical Science*, 2025, Volume 16, Number 18.
[3] *Quantum Technology Monitor 2025*, McKinsey, June 2025.
[4] "IonQ speeds quantum-accelerated drug development application with AstraZeneca, AWS, and NVIDIA," IonQ, June 9, 2025.
[5] "Advancing quantum chemistry in pharmaceuticals & agriculture with Boehringer Ingelheim," PsiQuantum, January 2025.

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Prediction of off-target effects. By creating more-precise simulations of reverse docking, QC can help identify potential side effects and toxicity early in development, reducing the risk of failures later in the process.

As these simulations become more accurate and reliable, they could significantly augment—or even replace, in some cases—aspects of clinical trials. By providing faster and more precise predictions of a drug's efficacy and safety in virtual human models, quantum computers could transform the R&D process, dramatically reducing the time and cost associated with bringing new therapies to patients.

Optimizing production and the supply chain

QC also offers significant opportunities in manufacturing and production. The optimization of pharmaceutical manufacturing facilities relies on a deep understanding of how complex molecules behave during transport and under varying environmental conditions. Current computational methods, such as the density functional theory, often lack the accuracy needed for modeling these dynamic, multicomponent systems. QC can provide more elaborate and precise simulations of questions such as crystallization processes, formulation stabilities, and biologics integrity during manufacturing and distribution, leading to significant improvements in yield, stability, and efficiency.

The synergy between QC and AI

QC can be combined with AI, classical computing, or both to achieve higher performance. For instance, quantitative structure–activity relationship models correlate structure and activity using shared properties of known molecules to make predictions for new ones. Insufficient training data renders the predictions unreliable and limits their applicability, but QC can generate training data to fill the gap.

Furthermore, the burgeoning field of quantum machine learning (QML) holds the promise of algorithms that can process high-dimensional data more efficiently, potentially optimizing the design of clinical trials and predicting patient responses to therapies. Researchers have recently developed a new liquid biopsy technique using QML, which distinguishes between exosomes—microscopic particles released by cells—from cancer patients and those from healthy individuals by analyzing their electrical "fingerprints."[6] This approach produces better predictions with minimal training data compared with classical methods, offering a faster, less invasive, and more cost-effective way to detect cancer sooner.[7] Additionally, Merck KGaA and Amgen are collaborating with QuEra to leverage QC for predicting the biological activity of drug candidates based on molecular descriptors.[8]

[6] "Quantum AI creates a better liquid biopsy for cancer," University of Chicago Pritzker Schol of Molecular Engineering, June 24, 2025.
[7] Abhimanyu Thakur et al., "Quantum machine learning-based electrokinetic mining for the identification of nanoparticles and exosomes with minimal training data," *Bioactive Materials*, September 2025, Volume 51.
[8] Daniel Beaulieu et al., "Robust quantum reservoir computing for molecular property prediction," arXiv, December 9, 2024.

The outlook for QC in life sciences

Although still in its early stages, the era of practical QC in life sciences is approaching rapidly. Leading pharmaceutical companies are exploring the possibilities, primarily through collaborations with pioneers in quantum technology. Besides those mentioned above, Amgen has used Quantinuum's QC capabilities to study peptide binding; IBM and Moderna have successfully simulated mRNA sequences using a hybrid quantum-classical approach; and Biogen is working with 1QBit to speed up molecule comparisons for neurological diseases such as Alzheimer's and Parkinson's.[9]

Although fully fault-tolerant quantum computers are still in development, road maps indicate that increasingly powerful and capable systems will emerge within the next two to five years, delivering practical applications and tangible, real-world benefits to the life sciences industry.

A road map to quantum value

For life sciences companies, the path to harnessing QC requires a deliberate and strategic approach, beginning with creating a clear road map:

— *Pinpoint the value*. Start by identifying the most pressing R&D and operational challenges, such as in target discovery or clinical trial efficiency, for which quantum's unique capabilities can create the greatest benefits.

— *Build strategic alliances*. Develop a network of partnerships with quantum technology leaders to ensure access to the latest hardware, software, and specialized knowledge.

— *Invest in human capital*. Recruit and cultivate a multidisciplinary team with expertise in computational biology, chemistry, and QC.

— *Future-proof your data strategy*. Establish a secure and scalable data infrastructure that can handle the outputs of quantum simulations and protect against the emerging threat of quantum decryption.

These steps can establish a strong competitive edge. Companies that invest early will be better positioned to not only accelerate their research and reduce costs but also deliver life-changing therapies more quickly to patients in the coming years.

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[9] Charles London et al., "Peptide binding classification on quantum computers," arXiv, November 27, 2023; Candace Gillhoolley, "IBM + Moderna: Using quantum to shape the future of mRNA therapies," Neurodiversity Marketing, July 26, 2025.