QUANDELA

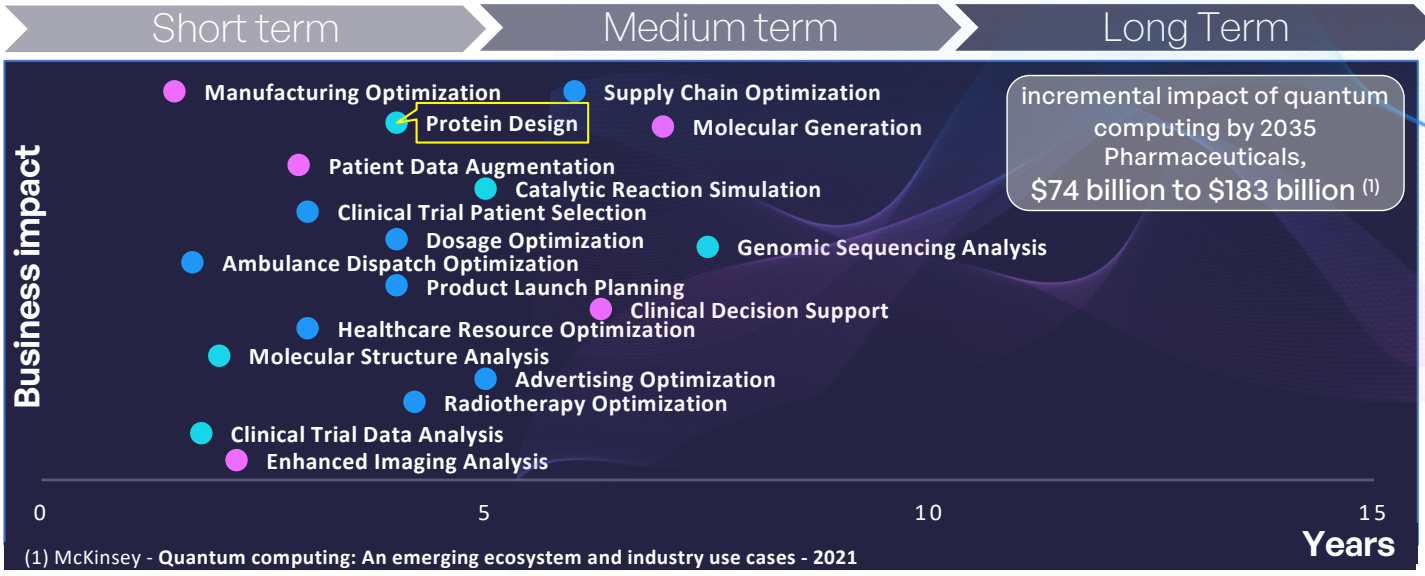
2023- Case story

Healthcare & Life Sciences

Biopharma drug discovery boosted by Quantum Simulation

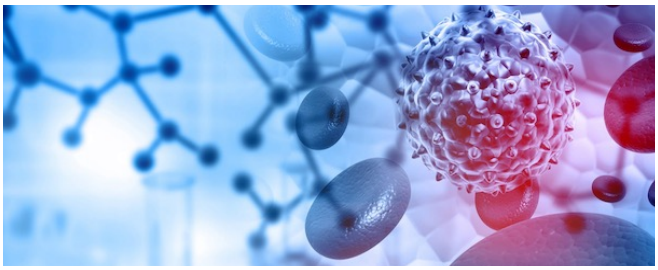
Use-cases for Healthcare & Life Sciences

Quantum Machine Learning	Molecular Generation, Genomic Sequencing Analysis, Enhanced Imaging Analysis, Patient Data Augmentation, Clinical Decision Support
Quantum Simulation	**Protein Design**, Molecular Structure Analysis, Catalytic Reaction Simulation, Clinical Trial Data Analysis, Supply Chain Optimization
Quantum Optimization	Clinical Trial Patient Selection, Dosage Optimization, Radiotherapy Optimization, Product Launch Planning, Manufacturing Optimization, Healthcare Resource Optimization, Advertising Optimization, Ambulance Dispatch Optimization



(1) McKinsey - **Quantum computing: An emerging ecosystem and industry use cases - 2021**

Challenge for Biopharma : increasing the R&D efficiency



The biopharma R&D process—from drug discovery to development—is a **costly (~ $180 billion/year)**[1], 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[1] for a single new drug. The success rate is less than 10% from entry into clinical development to launch.

In 2022, **Bio Artificial Intelligence market was estimated at $1.200 millions**[1]. High-performance computing is already key for drug discovery and development = modeling of molecular structures, mapping of the interactions between a drug and its target, simulations of the drug's metabolism, distribution, and interactions in the wider human system.

Next technical revolution should be **computational chemistry algorithms** aim to predict how a potential drug molecule will bind to specific target proteins, by modeling the binding energy of interaction.

(1) Source McKinsey

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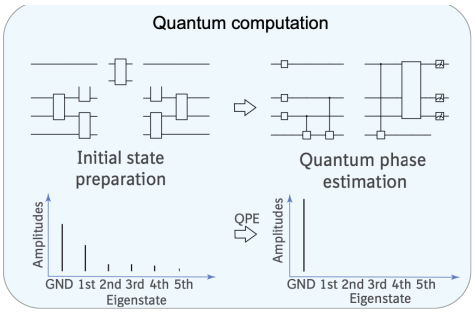
"Quantum computing is likely to have a profound impact on biopharma R&D, potentially changing the competitive set and dynamics of drug discovery."

BCG - Will Quantum Computing Transform Biopharma R&D?

"Quantum Computing's biggest impact on pharma will be in the discovery phases."

McKinsey - Pharma's digital Rx: Quantum computing in drug R&D

Solution : leverage Computer Assisted Drug Discovery (CADD)



Quantum Computing could make current CADD tools more effective by helping to **predict molecular properties with high accuracy.** That can affect the development process in several ways, such as modeling how proteins fold and how drug candidates interact with biologically relevant proteins. Here, QC may allow researchers to screen computational libraries against multiple possible structures of the target in parallel. Current approaches usually restrict the structural flexibility of the target molecule due to a lack of computational power and a limited amount of time. These restrictions may reduce the chances of identifying the best drug candidates.

In the longer term, Quantum Computing may improve generation and validation of hypotheses by using Machine Learning algorithms to uncover new structure-property relationships. Once it has reached sufficient maturity, QC technology may be able to create new types of drug-candidate libraries that are no longer restricted to small molecules but also include peptides and antibodies. It could also enable a more automated approach to drug discovery, in which a large structural library of biologically relevant targets is automatically screened against drug-like molecules via high-throughput approaches.

One could even envision QC triggering a paradigm shift in pharmaceutical R&D, moving beyond today's digitally enabled R&D toward simulation-based or in silico drug discoveries—**a trend that has been seen in other industries as well.**

Quantun Computing use cases apply to multiple aspects of drug discovery and will emerge at different points over an extended timeline. All of them, however, may enable more accurate and efficient development of targeted compounds.

To go further, read Raffaele Santagati et al., Drug design on quantum computers, https://arxiv.org/abs/2301.04114

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Consultation with Quantum scientists to explore the best approaches

Test and benchmark these approaches on state-of-the-art Quantum Processors (QPU)

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