

Integrating artificial intelligence (AI) into the drug discovery phase of pharmaceutical R&D

Capgemini brings a blend of data science, IT and science capabilities to unravel the high complexity in pharmaceutical R&D to enable more intelligent, value-driven innovation

The need for speed

The COVID-19 pandemic has shone a spotlight on the need for faster research and development (R&D) processes in life sciences. At the moment, bringing a new drug to market costs at least \$2 billion and can take up to 10 years, and the pharmaceutical industry is all too aware that drug discovery, trials and therapy launches are too complex, costly and slow: Life threatening viral diseases like COVID-19 and Ebola, have piled on the pressure to change this.

One of the world's large pharmaceutical companies wanted to use data science and AI to improve the route to market for new drug therapies. With the entire industry in the throes of transformation, and experiencing a turbulent market environment, the race was on to find new drugs and new indications for existing ones.

In order to ensure that it had access to the right tools to create value across the company's portfolio and development pipeline, the pharmaceutical client called upon its existing partnership with Capgemini to accelerate its shift towards faster and more connected AI-augmented drug discovery processes.

Overview

Client: A large, multinational biopharmaceutical company

Region: UK

Sector: Healthcare & Life Sciences

Client Challenge:

Like all companies in the healthcare industry, this global pharmaceutical giant was under tremendous pressure to reduce the time, cost and complexity involved in developing new drugs.

Solution:

Via a longstanding strategic partnership with Capgemini focusing on data science, through a variety of different yet connected projects the pharmaceutical company is increasingly integrating AI and machine learning into the discovery phase of drug development, to transform the process.

Benefits:

- Increase effectiveness of drugs discovered, and value from the drug discovery process
- Remove cost, time and inefficiencies from the drug discovery process
- Provide research teams' intuitive access to innovative technologies that maximize their scientific expertise



Advancing discovery

The lead discovery phase of drug development involves working to find candidate molecules that will be effective in treating a disease, a complex process involving vast scales of potential data: the number of small molecule candidates available for drug design is up to 1060. The pharmaceutical company worked with Capgemini to create and apply new machine learning methods to improve 'cheminformatics': the computational and mathematical techniques involved in analysing collections of molecules and their properties. By combining broad AI expertise with deep subject matter knowledge, it was possible to apply techniques from seemingly unrelated areas to solve pharmaceutical R&D challenges in computational drug modelling.

One such project involved harnessing the neural networks behind cutting-edge language translation methods to help establish new molecules with the potential to have the right drug-like properties and biological activity. Working together, the organization and Capgemini were able to apply language translation techniques to 'translate' the outline of an existing molecule into a new one to generate candidates that match requirements. This [ground-breaking approach](#) uses machine learning techniques to guide the design and refinement of these molecules.

A second project focused on the simplification and acceleration of research workflow. Inconsistent interfaces and varying data requirements between the many different tools for the computer simulation of the chemical space of molecules, and their interactions with proteins, can make it hard for the scientific community to use and maintain the associated technologies. To solve this problem, the pharmaceutical company and Capgemini created a system that combines the entire spectrum of tools, for generating molecules, making predictions and designing experiments. This enables researchers to combine their scientific expertise with AI techniques without needing deep technical knowledge of the system itself.

An intelligent future

These are just two examples of how the pharmaceutical company and Capgemini have used AI to improve efficiencies, address complexity and more quickly innovate to create value. This includes not only looking for new molecular solutions but also for the potential to adapt existing drugs for new uses. Using AI for predictive modelling at the early stages of drug development allows researchers to examine more molecular variations while accelerating prioritization. And this has the potential to transform drug discovery: increasing the effectiveness of what is developed, and cutting cost, time and inefficiencies from the entire process. In doing so, the partnership is demonstrating that AI provides a more effective and trustworthy means of obtaining more value from complex data at scale.





About Capgemini

A global leader in consulting, technology services and digital transformation, Capgemini is at the forefront of innovation to address the entire breadth of clients' opportunities in the evolving world of cloud, digital and platforms. Building on its strong 50-year heritage and deep industry-specific expertise, Capgemini enables organizations to realize their business ambitions through an array of services from strategy to operations. Capgemini is driven by the conviction that the business value of technology comes from and through people. It is a multicultural company of over 270,000 team members in almost 50 countries. With Altran, the Group reported 2019 combined revenues of €17 billion.

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