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Artificial intelligence in drug discovery

The effects of artificial intelligence on the drug-discovery process

What is artificial intelligence?

Artificial intelligence (AI) is the ability of a machine to exhibit human-like intelligence. Computer science and large, robust datasets are used to develop the algorithms that can mimic the cognitive functions of humans; they can learn, solve problems, identify patterns and generate predictions.

AI is often referred to as narrow or general AI (AGI). Narrow AI focuses on performing specific tasks extremely well, whereas AGI can learn and solve problems in any environment. Narrow AI is ubiquitous (Google search, Amazon's Alexa), but AGI is only hypothetical.

Narrow AI is trained to solve problems and adapt to change using the concept of machine learning. AI algorithms analyse previous actions and can autonomously improve when given new datasets. As a result, the AI can become more accurate.

Which specific drug discovery challenges can AI solve?

AI can analyse vast quantities of data, allowing it to identify patterns in datasets that are too complex for humans to discern. It can also generate predictions based on these data, potentially leading to the rapid and accurate identification of novel drug targets and lead molecules. AI can also use natural language processing to bring together disparate information and datasets, providing researchers with insights that no single experiment could provide.

One of the key challenges in drug discovery is understanding the structure of the protein that a drug could target. Although structures can be discerned experimentally, the process is time consuming and expensive. Google's DeepMind has recently launched AlphaFold, an AI platform that can predict protein structures with high accuracy. Alphafold has provided a solution to one of the key bottlenecks in drug discovery, enabling a vast new set of potential drug targets to explore.

Biological systems consist of highly complex networks of interactions. The complexity of the system makes it difficult to predict how a drug will have adverse effects. E-therapeutics use AI to model and analyse these complex networks, and hypothesise that a representative simulation of a whole biological system will help translate therapies from laboratory to patient, reducing expensive clinical-stage failure.

Which companies are using AI in drug discovery and who is backing them?

The potential for a faster and cheaper age of drug discovery has led to the founding of numerous start-ups over the last decade. Many have raised large amounts of investment and established partnerships with large biopharma companies.

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'Despite its infancy, AI is broadly being touted to have a revolutionary effect on the drug discovery process, with potential to mitigate attrition, accelerate development timelines or reduce cost. On the back of this promise, a plethora of partnerships have been struck between AI-vendors and drug developers, along with a spate of fundraising for AI-based drug discovery platforms.' Sean Conroy, healthcare analyst

Exscientia has developed an automated AI platform that has multiple functions throughout the drug-discovery process. The platform can scour literature to find drug targets that would not be obvious to humans. It has also demonstrated the ability to optimise drugs better than humans. Using this platform, it became the first company to successfully progress a fully AI-designed drug candidate into Phase I clinical trials. In April, Exscientia announced its second drug candidate entered the clinic, an A2a receptor antagonist which was identified within just eight months of project initiation. Exscientia claims this process would typically take four to five years, but the use of its AI platform significantly shortened the process. Exscientia floated on Nasdaq in October, raising $510m in aggregate financing, with

SoftBank, BMS, Evotec and Novo all notable shareholders.

BenevolentAI creates 'knowledge graphs' using machine learning to connect related biomedical data from its large repository. The knowledge graphs contain insights that humans would not be able to synthesise alone, due to the complexity and volume of the data. The information can be used to identify drug targets, develop lead molecules and repurpose known drugs. BenevolentAI identified that baricitinib (an approved rheumatoid arthritis drug) had potential to be used in the treatment of COVID-19. The FDA subsequently authorised the use of baricitinib to treat hospitalised COVID-19 patients. BenevolentAI is in collaboration with AstraZeneca and the partnership combines BenevolentAI's platform with AstraZeneca's expertise and large datasets. In January, it announced the discovery of a novel target for chronic kidney disease.

Recursion aims to make drug discovery faster and cheaper using machine vision to identify subtle changes in cell biology, caused by the treatment of molecules. The approach allows the company to rapidly analyse vast quantities of experimental data. The data are generated in-house using its automated robotic laboratory, which perform 1.5 million experiments each week. The company has four drug candidates in Phase I clinical trials and has an ongoing partnership with Bayer that aims to develop new therapies in fibrotic disease. Recursion completed its US$436m IPO on Nasdaq in April.

Will the pharmaceutical industry's use of AI continue?

Overall, the discovery of a new drug is estimated to cost over US$2.6bn and take at least 10 years. Although the AI technology is still nascent and applications are being explored, it is thought AI could be used at numerous stages of the drug discovery process.

There is broad recognition of the potential of AI to improve the drug discovery process. Since 2015 there have been around 100 new partnerships between AI services and the pharmaceutical industry. Additionally, in November, Alphabet announced the launch of Isomorphic Labs, a spin-off of DeepMind, which aims to deliver an 'AI-first approach' to drug discovery.