

HEADING

Artificial intelligence

AI-designed drug to enter human clinical trial for first time

Molecule designed by machine to treat OCD developed in just 12 months

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A drug molecule invented entirely by artificial intelligence is set to enter human clinical trials for the first time, marking a critical milestone for the role of machine learning in medicine.

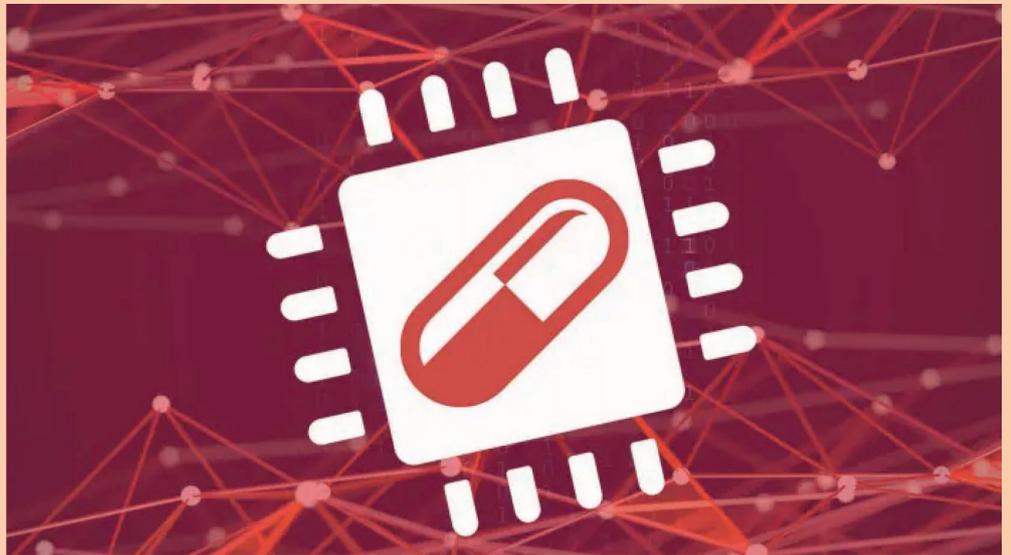
The new compound, which has been designed to treat patients with obsessive-compulsive disorder, was developed by Oxford-based AI start-up Exscientia in collaboration with the Japanese pharmaceutical firm Sumitomo Dainippon Pharma.

In a sharp acceleration of the typical path to drug development, which can take about four and a half years, the AI-designed compound reached the point of entering clinical trials within just 12 months.

The breakthrough comes at a time when investors are pouring billions of dollars into companies that are accelerating drug development using AI. On average it costs about \$2.6bn to develop a new treatment by traditional methods, but the use of AI could make drug discovery faster, cheaper and more effective for patients with a range of illnesses from cancers to heart disease.

So far, machine learning algorithms, combined with troves of patient data, have been used to successfully expand the number and types of patients who can benefit from existing medicines. But the invention of entirely new drugs by AI that are both clinically safe and effective in humans has been harder to achieve.

“The design and development of molecules through medicinal chemistry has always been a slow and laborious process,” said Sir John Bell, the Regius professor of medicine at Oxford university, who was not involved with



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the research. “Exscientia can do this in many fewer steps, which is really impressive, and it comes from very sound scientific principles. I think they are a real asset to have in the UK.”

Exscientia’s AI platform used a suite of algorithms to decide on the best chemical structure for the new compound, which is known as DSP-1181 and is targeted at a specific receptor in the brain involved in OCD. Together the algorithms were able to generate tens of millions of potential

molecules, sift through the candidates and make a decision about which ones to synthesise and test.

“The AI can learn faster than conventional approaches, so we had to make and test only 350 compounds, a fifth of the normal number of compound candidates, which is record-breaking productivity,” said Andrew Hopkins, chief executive of the start-up and a molecular biophysicist.

“The algorithms . . . can be applied to any drug targets, against a huge range of diseases in oncology, cardiovascular and rare diseases.”

The 60-person start-up is working with other pharmaceutical companies including Bayer and Sanofi to design new drugs for other conditions such as metabolic disease, and has raised \$43m from Bristol-Myers Squibb, among others.

Toru Kimura, senior executive research director of Sumitomo Dainippon Pharma, added: “We are very excited with the results of the joint research . . . We will continue to work hard to make this clinical study a success so that it may deliver new benefits to patients as soon as possible.”

Additional reporting by Sarah Neville