Using AI for drug discovery shows speed but draws discussions

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A drug molecule developed though machine learning? An <u>announcement</u> has been made that a phase I clinical study of DSP-1181, that was created using Artificial Intelligence (AI), has been initiated in Japan.

This project required less than 12 months to complete "the exploratory

research phase," and this represents "a fraction of the typical average of 4.5 years using conventional research techniques," said the company release.

If you can possibly wrap your arms around this: It is invented by artificial intelligence. Certainly a sign that progress can be watched for the potential of machine intelligence in discovering drugs?

BBC technology reporter Jane Wakefield reported there are two groups behind this advance, (1) British start-up Exscientia and (2) Japanese pharmaceutical firm Sumitomo Dainippon Pharma. (Psychiatry and neurology are among the latter company's key focus areas for research).

She said that the drug will be used to treat patients who have obsessive-compulsive disorder (OCD).

Exscientia said that it is a company "at the forefront of Artificial Intelligence-driven drug discovery and design." They feel that they have reached "a critical milestone" in the development of AI and medicine.

They pointed to their AI advantage regarding the pre-clinical drug discovery stage—resulting in the potential to speed up the delivery of new treatments.

After all, consider that "it takes around 10 to 15 years for a drug to go from initial discovery to the marketplace. That's too long," they remarked.

They described themselves further on their site as "a full stack AI drug discovery company."

Meaning what? Specifically, they generate their own data "before combining the analytical power of AI with the creativity and expertise of

our world-class scientists."

Interestingly, it was back in [December](link) when *Nature* posed a question about AI in medicine. "The pharmaceutical industry is in a drug-discovery slump. How much can AI help?"

The article by David Freedman said "the $1-trillion global [pharmaceutical industry](link) has been in a [drug development](link) and productivity slide for at least two decades. Pharmaceutical companies are spending more and more—the 10 largest ones now pay nearly $80 billion a year—to come up with fewer and fewer successful drugs."

What is the snag? Freedman said, "drugs that are easiest to find and that safely and effectively treat common disorders have all been found; what is left is hunting for drugs that address problems with complex and elusive solutions..."

Freedman's description of how scientists use AI tools for drug development was instructive: "These tools do not work by having expert-developed analytical techniques programmed into them; rather users feed them sample problems (a molecule) and solutions (how the molecule ultimately behaves as a drug) so that the software can develop its own computational approaches for producing those same solutions."

BBC said that the molecule DSP-1181 was achieved through algorithms that sifted through potential compounds. These were checked against a "huge" database of parameters.

[Recode](link) reporter Rebecca Heilweil helped clarify what this checking against parameters meant for researchers:

"There are lots and lots of possible molecules that might be useful in medications, far too many for all the medical researchers in the world to

manually test. But by using different types of AI, a computer system can come up with and mine through different molecules, comparing them against different parameters and learning the most promising compounds faster than a human could."

Just as artificial intelligence in general has sparked calls for caution and review in fields other than medicine, it is reasonable to expect similar thoughts regarding drug discovery.

A headline in *Recode* gives you a hint of the discussions ahead. "Would you take a drug discovered by artificial intelligence?"

"Artificial intelligence is certainly powerful, wrote Heilweil, "but some are skeptical that the technology is reliable...and question what role it should play in areas like our health care. And in drug research, some have voiced concerns that the technology might be overhyped."

The press release coming out of Exscientia specifically talks about DSP-1181 as a phase I clinical study that has been initiated in Japan for the treatment of obsessive-compulsive disorder as an initial indication.

All in all, we get it. AI is going to serve a significant role in drug discovery breakthroughs ...or will it?

Science Translational Medicine ran an editorially independent commentary on Jan. 31 by Derek Lowe It's an independent blog from the publishers. He's worked for several major pharmaceutical companies on drug discovery projects. He posed questions about what we consider a drug discovery revolution.

The commentary noted that this took one year to get into the clinic. "If that's accurate, that is indeed a fast path into human trials, but let's look at what that might get you. Will this be a drug discovery revolution?" he

asked.

Lowe, then, was not arguing about the speed edge. "Exscientia may well have moved a compound along at high speed into the clinic. But this particular example is not going to accelerate drug discovery much."

Consider, he said, the information that is fed into the software. "There is simply not enough reliable information to feed into even the greatest artificial intelligence software in the world to allow one to predict what will happen against conditions like OCD, depression, anxiety, and other high-level human psychiatric conditions," he argued. "And that is the problem. Drugs fail in Phase II because we have not picked the right target, because our biochemical understanding of the disease state is wrong and/or incomplete."

One of the reader comments reacting to his commentary did not challenge his points but did maintain that the AI company announcement still marked progress.

"While I agree w/ Derek that there's a lot of overhype around the 'AI in drug discovery space,' said one comment, "that doesn't mean that there aren't real tangible gains being made here as well... So even if this is incremental progress, increased efficiencies from new technologies, even against known targets or potentially derivative chemical matter, should be welcomed with open, if rightfully skeptical, arms… This isn't a magic wand, it's another tool in the toolbox."

Heilweil wrote that "As remarkable as the new drug's development seems, there's still room for some healthy skepticism." She said, "the development of AI-assisted pharmaceuticals raises questions about how comfortable people should be with these new research methods. In the long run, how will AI-designed drugs differ from those developed by humans alone? Who should make the rules for the use of AI in drug

research?

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