How AI is shaping clinical research and trials

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Artificial intelligence (AI) is everywhere at the minute, seemingly being used in some capacity in almost every professional industry, including clinical research and trials.

In fact, it is fair to say that AI has taken the biotech industry by storm, and the hype surrounding it has led to numerous AI startup companies coming onto the scene, using AI for everything from diagnostics to drug discovery and development. Even ChatGPT has been integrated into certain companies' drug discovery processes.

As so many people within the industry have discovered, AI brings with it a whole load of benefits, and making the most of the opportunity it presents can lead to faster success stories and milestone achievements in clinical research, including clinical trials.

For example, a couple of months ago, AI helped scientists to discover a new antibiotic called abaucin, which can kill *Acinetobacter baumannii,* a superbug that causes fever, chills, and vomiting. It also happens to be multi-drug resistant.

In this instance, AI was able to rapidly screen 7,500 molecules that were found to inhibit *A. baumannii*, and in one and a half hours it managed to narrow down 250 potential compounds, after which abaucin was found to be the most potent one.

Manually, this task would have been extremely difficult. But, by using AI, the entire process was sped up, meaning the antibiotic discovered could end up being used to treat *A. baumannii* a lot sooner than if the process had been done manually, which ultimately could be life-saving for people in the near future.

What are the advantages of using AI in clinical research?

Of course, as mentioned, speed is one of the key advantages of using AI in clinical research and trials.

This is extremely significant, as, according to research from the Deloitte Centre for Health Solutions, it can often take 10 to 12 years to bring a new drug to the market, and the clinical trial stage itself averages five to seven years, largely thanks to the complications of manual effort, rework, and inefficiency.

"The time frame for developing a new drug from ground zero takes about 10 to 12 years, using $1.2 billion in a very conservative estimate. With AI, you can shorten it easily by more than half, to about 5 years. That's what we are seeing today. A lot of people in drug development will agree with that, especially for drug discovery to get the right drug and go to the next stage," said Gideon Ho, co-founder and chief executive officer (CEO) of HistoIndex, a company using AI coupled with stain-free pathology to look at biopsy samples without staining the tissue, before using a laser to scan and image the biopsy, and employing AI for data readout to assess the magnitude of treatment efficacy for fibrotic diseases.

As well as speed, Ho also listed consistency, accuracy, repeatability, and scalability as the main advantages of using AI in the life sciences industry.

"These are highly important as they can augment areas and be applied anywhere from drug discovery, to drug testing in preclinical animal models, safety and toxicity testing, assessment of efficacy during human clinical trials and even FDA approvals of the drug itself," he said.

Ho estimated that AI is being used in around 50% to 60% of the entire value chain of drug development. And, not only is AI being used for drug discovery, it can also also be used in the following stage, which involves testing the discovered molecule in pre-clinical animal or in vitro models, or in safety testing or assessment of the efficacy of drugs in human trials.

Essentially, AI can be used across pretty much the entire drug development process.

AI for drug design

AI is being used more and more in preclinical and clinical trials, with advanced algorithms able to rapidly analyze vast databases of chemical compounds and identify the ones that are most likely to bind to a target, enabling drug developers to explore the chemical world far more quickly.

IKTOS is a company making use of AI technology specifically for drug design, using it to rapidly identify molecules – in this case, the company focuses on small molecules – that are suitable to become clinical candidates.

Company CEO, Yann Gaston-Mathé, explained the drug design process: "So, essentially, when you do small molecule drug discovery, you start with your target...we usually start by screening libraries of known molecules on this biological assay, then identifying what's called a 'hit' – a hit being a molecule which is active in your biological assay – and then once you have a hit, you will start doing some chemistry, meaning you will modify the hit in order to improve the level of activity or the potency and also progressively optimize the molecule in order to make it selective on your target."

Ultimately what you want to end up with is a molecule that is active, selective, has no toxicity, and is novel.

And, once again, the reasoning behind wanting to use AI for this process is essentially all about saving time, as it requires the synthesizing and testing of thousands of molecules. Done manually, it would take years of research, and the cost would be enormous.

But, using its AI technology, IKTOS can go about the process of designing drugs far more quickly and efficiently, designing new molecules automatically.

First fully AI-generated drug enters clinical trials

In another recent success story for AI in clinical research, it was announced that the first fully AI-generated drug had entered clinical trials in humans.

The drug, INS018_055, is being developed by Hong-Kong based Insilico Medicine and has reached phase 2 trials for the treatment of idiopathic pulmonary fibrosis – a chronic disease that causes scarring in the lungs and makes breathing increasingly difficult.

The company connects biology, chemistry and clinical trial analysis using next-generation AI systems, having developed AI platforms that use deep generative models, reinforcement learning, transformers, plus other modern machine learning techniques. They are used for novel target discovery and the generation of novel molecular structures that have desired properties.

And, although there have been other AI-designed drugs in clinical trials, INS018_055 is the first drug with both a novel AI-discovered target, as well as a novel AI-generated design.

Insilico Medicine also has two more drugs in the clinical stage that have been partially generated by AI; one for COVID-19 in phase 1 trials, and the other solid tumors that recently received approval from the U.S. Food and Drug Administration (FDA) to initiate clinical trials.

What is the future of AI in clinical research?

The use of AI in clinical research has really taken off in recent times, and with the technology seemingly advancing at breakneck speed, it's likely that AI will take on more and more responsibilities in the drug development process in order to guarantee speed and efficiency.

"I would say that it is going to be AI inserting itself into different parts of the entire drug development process, as an aiding tool into the entire diagnostic process, in decision-making by the clinicians to make better decisions...," commented Ho.

Additionally, the hype around AI is even expected to kick off a resurgence of investment into the biotech industry, after a difficult economic period in which companies have struggled to raise capital.

All in all, it seems like AI is the future of clinical research and trials in the life sciences industry, and Ho believes that people within the industry should embrace it as the useful tool that it is. "The people who use AI will definitely replace people who don't use AI. It's a natural evolution of things. If you have new tools and you do not use them, you're basically rendering yourself basically obsolete. If it is a good tool, we should use it and embrace it so that we will continue to remain relevant to the industry."

And, with the amount of AI startups and technology around at the minute, it's fair to say that people in the industry *are* indeed embracing it.