Quicker Cures: How Insilico Medicine Uses Generative AI to Accelerate Drug Discovery

The startup, a premier member of NVIDIA Inception, is entering Phase 2 clinical trials with a drug candidate discovered using its AI platform.

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While generative AI is a relatively new household term, drug discovery company Insilico Medicine has been using it for years to develop new therapies for debilitating diseases.

The company's early bet on deep learning is bearing fruit — a drug candidate discovered using its AI platform is now entering Phase 2 clinical trials to treat idiopathic pulmonary fibrosis, a relatively rare respiratory disease that causes progressive decline in lung function.

Insilico used generative AI for each step of the preclinical drug discovery process: to identify a molecule that a drug compound could target, generate novel drug candidates, gauge how well these candidates would bind with the target, and even predict the outcome of clinical trials.

Doing this using traditional methods would have cost more than $400 million and taken up to six years . But with generative AI, Insilico accomplished them for one-tenth of the cost and one-third of the time — reaching the first phase of clinical trials just two and a half years after beginning the project.

"This first drug candidate that's going to Phase 2 is a true highlight of our end-to-end approach to bridge biology and chemistry with deep learning," said Alex Zhavoronkov, CEO of Insilico Medicine. "This is a significant milestone not only for us, but for everyone in the field of AI-accelerated drug discovery."

Insilico is a premier member of NVIDIA Inception , a free program that provides cutting-edge startups with technical training, go-to-market support and AI platform guidance. The company uses NVIDIA Tensor Core GPUs in its generative AI drug design engine, Chemistry42, to generate novel molecular structures — and was one of the first adopters of an early precursor to NVIDIA DGX systems in 2015.

Insilico's Pharma.AI platform includes multiple AI models trained on millions of data samples for a range of tasks. One AI tool, PandaOmics, rapidly identifies and prioritizes targets that play a significant role in a disease's effectiveness — like the infamous spike protein on the virus that causes COVID-19.

The Chemistry42 engine can design within days new potential drug compounds that target the protein identified using PandaOmics. The generative chemistry tool uses deep learning to come up with drug-like molecular structures from scratch.

"Typically, AI companies in drug discovery focus either on biology or on chemistry," said Petrina Kamya, head of AI platforms at Insilico. "From the start, Insilico has been applying the same deep learning approach to both fields, using AI both to discover drug targets and generate chemical structures of small molecules."

Over the years, the Insilico team has adopted different kinds of deep neural networks for drug discovery, including generative adversarial networks and transformer models . They're now using NVIDIA BioNeMo to accelerate the early drug discovery process with generative AI.

To develop its pulmonary fibrosis drug candidate, Insilico used Pharma.AI to design and synthesize about 80 molecules, achieving unprecedented success rates for preclinical drug candidates. The process — from identifying the target to nominating a promising drug candidate for trials — took under 18 months.

During Phase 2 clinical trials, Insilico's pulmonary fibrosis drug will be tested in several hundred people with the condition in the U.S. and China. The process will take several months — but in parallel, the company has more than 30 programs in the pipeline to target other diseases, including a number of cancer drugs .

"When we first presented our results, people just did not believe that generative AI systems could achieve this level of diversity, novelty and accuracy," said Zhavoronkov. "Now that we have an entire pipeline of promising drug candidates, people are realizing that this actually works."

Learn more about Insilico Medicine's Chemistry42 platform for AI-accelerated drug candidate screening in this talk from NVIDIA GTC .

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