

## Emerging Space Brief

# AI-Powered Drug Discovery

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## Top companies by total VC raised



## Contact

### Research

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## Overview

Companies in this space leverage artificial intelligence (AI) to research and discover new pharmaceuticals and drug therapies. AI systems sift through millions of chemical compounds and isolate the most promising candidates in a fraction of the time it would take human researchers. Though an AI-created drug has yet to be put to market, proponents hope that upcoming technological advances might expedite drug development timelines and enable pharmaceutical companies to develop drugs in previously unprofitable areas.

## Applications

### Target proteins

Some AI companies, for example, focus on designing a drug that can safely and effectively work on a known target—usually a specific, well-studied protein that is linked to a disease. Companies hope to come up with a molecule that chemically binds to the target protein and then modifies it to prevent further contribution to the disease or the symptoms. A Canadian firm, Cyclica, develops software that matches both biophysical structures and biochemical properties of millions of molecules to the structures and properties of around 150,000 proteins in an effort to find the molecules most likely to bind with target proteins.<sup>1</sup>

## Technologies & processes

### Machine learning

Machine learning (ML), as well as ML subset deep learning, are popular techniques in this space. ML programs ingest small amounts of data that have been annotated with the help of human expertise, whereas deep learning programs ingest unstructured data sets in large volumes. The approach used depends on the

<sup>1</sup> "Hunting for New Drugs with AI," David H. Freedman, *nature*, December 18, 2019.

amount of data available. For example, in cases with only a few thousand annotated examples, ML is relied upon. However, if there is enough raw data, it can be fed into a deep learning program, which can learn and process the data without the annotation.

### Big Data

Given the constraints of ML, Big Data plays a huge role in the potential success of AI-powered drug discovery. With this technology's acceleration, many researchers are changing the outputs of their studies—such that the resulting data is plentiful enough to justify using a deep learning program. Ideally, AI-driven results will allow researchers to better target their future research, which in turn will provide new data that can be fed into an ML program.

## Outlook

### Technological learning curve

While most in the pharmaceutical industry feel optimistic that these tools will provide an edge, many still wonder how such technologies will deliver on their promises. Some in the scientific community feel frustrated by the overblown ambitions of tech companies. They worry that too much overpromising could lead to a public mistrust of the technology and a thaw in funding that would stall productivity. Much experimentation remains to determine where AI can have the most impact in the drug discovery pipeline and where its current promises may be overblown.

### Restoring productivity

Drug development and productivity in the pharmaceutical industry has diminished over the past two decades, with large pharma companies spending nearly \$80 billion per year to develop fewer successful drugs. According to *Scientific American*, 10 years ago, every dollar invested in research development had a return of 10 cents. Today, the return is two cents, in part because the drugs that are easiest to find and use for treatments have seemingly all been identified. A complex web of specialized diseases and disorders remains, making research more time-intensive and, by extension, more costly. By testing the candidates through an AI program, researchers can save time. One estimate posits that these programs could shave five years off the usual seven-year time frame for bringing a candidate drug to human trials.<sup>2</sup>

### Big Pharma already embraces AI

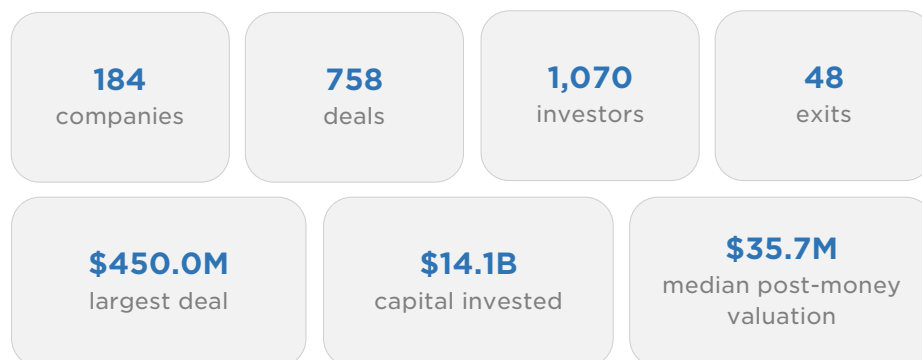
At least 20 partnerships have been reported between pharmaceutical companies and AI drug discovery startups. Some of the key incumbents, such as Pfizer (NYSE:

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<sup>2</sup> ["Hunting for New Drugs with AI," David H. Freedman, nature, December 18, 2019.](#)

PFE), GlaxoSmithKline (LON: GSK), and Novartis (SWX: NOVN), are all developing in-house AI expertise. Many others will likely follow their lead.

### Quantitative perspective



\*As of November 4, 2021

### Recommended reading

["How Artificial Intelligence Is Changing Drug Discovery," Nature, Nic Fleming, May 30, 2018.](#)

["Hunting for New Drugs with AI," Scientific American, David H. Freedman, February 1, 2020.](#)

["How Big Pharma Adopts AI to Boost Drug Discovery," BiopharmaTrend, Andrii Buvailo, October 8, 2018.](#)

["Intelligent Drug Discovery: Powered by AI," Deloitte Centre for Health Solutions, 2019.](#)