



CONNECT

Smart drug discovery

Background

Artificial intelligence is becoming increasingly tangible. There are different types of AI, with machine learning being the most common. In healthcare, AI can enable previously untapped opportunities - for example, in drug discovery. Did you know that it costs around \$2.6 billion to bring a new drug to market these days? And not only is the process costly: ultimately, only 10 percent of drug candidates make it to market after Phase 1 trials, which also represents a high economic risk for companies.

Amazing opportunities through AI

Drug discovery relies on combining a continuously growing number of potential compounds in such a way as to achieve drug optimization. To make this possible, it is necessary to handle huge amounts of data effectively and accurately, which is where AI has emerged as an optimal partner. Large amounts of machine-readable data not only offer drug R&D the opportunity to gain new insights, but at the same time pose a major challenge as the derivation of insights becomes increasingly difficult due to the increasing amount of data. Another challenge is that it is also becoming increasingly difficult to maintain a holistic overview of the most important changes and developments in adjacent research areas, which should not go unnoticed, especially in drug development. Nevertheless, according to recent studies, around 80 percent of medical data remains unused after it has been collected.

The research and development of drugs pose a problem that can be solved by means of intelligent automation. From the multitude of possible combinations of drug molecules, an exciting optimization problem for AI applications is created with the goal of identifying possible lead compounds and validating the drug target as well as the design of the drug structure. In this way, it was also possible to identify potential Covid-19 treatments within a short period of time. Here, for example, a drug regularly used to treat rheumatoid arthritis was identified to combat viral inflammatory responses. For the first time, AI was brought in to solve a new problem based on an existing drug.

The benefits of intelligent automation have now been recognized and turned to advantage by a number of companies. One example is Pfizer, which in 2020 was not yet able to automatically search its library, which contains data on some 4.5 billion commercially available compounds. As of today, the company is able to search their entire database in a 48-hour period, significantly speeding up the identification of potential new drugs.

Results show that more than 40 percent of drug discovery startups are using AI applications to search chemical repositories for potential drug candidates. Another 28 percent are using AI to identify new targets and 17 percent are using it to map a computer-aided molecular design. It is



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expected that within the next 10 years, all major pharmaceutical companies will have integrated AI as an integral part of drug discovery.

Nevertheless, it is important to adopt a rational expectation and not propagate the misconception that AI could replace human expertise. AI should be used to support subject matter experts in the future, yet it must be controlled. Subject matter experts will continue to be the point of contact for defining data for AI analysis and for end-to-end verification of results.

As a result, it can be said that automation will play an important role in drug discovery and in the overall drug development process in the future. With the right balance between humans and machines, as well as reliable controls to strictly adhere to the task at hand, AI will play a crucial role in new drug discovery.

Want to learn more about collaborations between pharma and IT companies? We have researched for you and found a number of exciting mergers. See for yourself.

IT COMPANY	PHARMACEUTICAL COMPANY	FIELD OF EXPERTISE
IBM Corp.	Pfizer Inc.	drug discovery
Microsoft Corp.	Novartis AG	drug discovery
Nvidia Corp.	AstraZeneca Plc.	drug discovery
Exscientia Ltd.	Sanofi-Aventis	drug discovery
Owkin Inc.	Roche Holding AG	drug discovery
Exscientia Ltd.	Bayer AG	drug discovery
Google Quantum AI	Boehringer Ingelheim International GmbH	drug discovery

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