Power of AI: to identify better drug targets and drug candidates

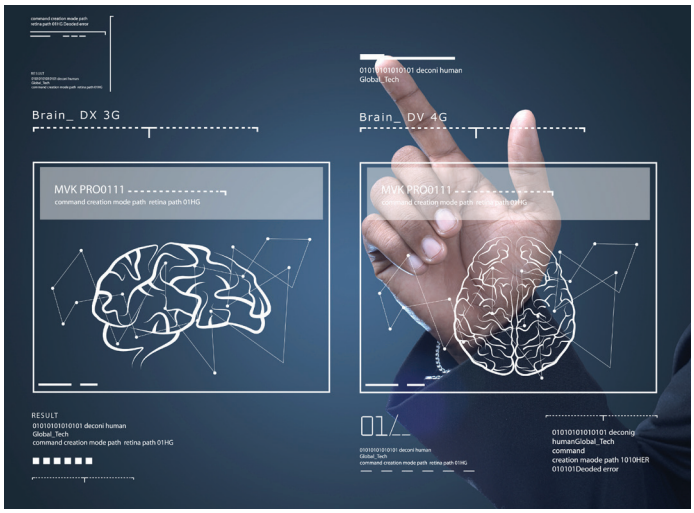
15 July 2023 | By **Dr. Mahesh Bhalgat**

https://health.economictimes.indiatimes.com/news/health-it/power-of-ai-to-identify-better-drug-targets-and-drug-candidates/101775248

AI helps identify better targets and candidates for drug development faster by utilising large datasets of biological and chemical information and applying machine learning algorithms to analyse the data.

The world has been taken over recently by OpenAI's platforms, ChatGPT-3 and 4, which can mimic human intelligence. The pharmaceutical industry is also witnessing a revolution in using Artificial Intelligence (AI) tools for drug discovery and development. Computational approaches have shifted the early-stage drug discovery process from serendipitous discovery to rational discovery to intuitive discovery, which makes the process more streamlined, effective, and efficient. Using the available data, AI and machine learning (ML) can understand the steps better, empowering scientists to move from data to decisions, faster.

Traditionally, drug discovery has been a time-consuming process of 10–15 years, costing more than US$2 billion to bring a new drug to market. Several factors lead to drug candidates being eliminated during the phase of drug discovery and development. As an example, undesirable pharmacokinetics and toxicity are significant reasons for unsuccessful drug development. AI and data-driven R&D processes can help anticipate and eliminate some of these issues resulting in a shorter timeline for drug discovery, lesser attrition during development, cheaper and more efficient than ever before. Morgan Stanley research mentions that improvements in early-stage drug development utilising AI and ML over the next decade could result in 50 new therapies with a $50 billion market. This article will explore the benefits of AI tools and how they can transform drug discovery and development.



How AI helps identify better targets and candidates faster

AI helps identify better targets and candidates for drug development faster by utilising large datasets of biological and chemical information and applying machine learning algorithms to analyse the data. AI can:

- provide a quicker validation of the drug target
- identify and design hit and lead compounds
- optimise drug design

AI models have helped identify potential anticancer targets and the discovery of novel drug candidates. These algorithms can identify drug candidates that are likely to have the

desired drug properties in terms of target specificity, potency, and pharmacokinetics, thereby reducing the number of drug candidates that need to be synthesised and tested in the laboratories.

Open databases, such as UniProt, DrugBank, ChEMBL, and PubChem, also play a critical role in drug discovery. These databases provide researchers with access to large amounts of biological and chemical data, which can be used to recognise potential drug targets and predict drug efficacy. By making this data available to researchers worldwide, open and public databases enable collaboration and accelerate drug discovery.

In recent years, *in silico* technology has been widely used to evaluate the relevant properties of drugs at the preclinical stage and has produced many software programs and models, promoting the study of ADMET (absorption, distribution, metabolism, and excretion) *in vitro* (2)

Similarly, AI approaches, such as deep learning and relevant modeling studies, can be implemented for safety and efficacy evaluations of drug molecules. Merck supported a Quantitative structure-activity relationship (QSAR) based computational model, which showed significant predictivity for 15 absorption, distribution, metabolism, excretion, and toxicity (ADMET) data sets of drug candidates.

Putting such tools with good predictive power requires many items to come together. High quality data is at the center of that along with a very good understanding of the underlying biology and a multidisciplinary team. Typically, the latter incudes a group of scientists with expertise across computational biology, computational chemistry, data sciences and research informatics is needed for all the research and development work. In the future, these tools can evolve such that a team of chemists and biologists can conduct the desired studies based on AI/ML without relying on bioinformaticists.

Pfizer is using AI to help revolutionise the development of life-saving drugs. The company is making advances in the biology of various diseases and is using the insights to identify molecules that can potentially treat diseases. Atomwise, has established a research collaboration with Sanofi that will leverage its AtomNet® platform for computational discovery and research of up to five drug targets. The AtomNet platform incorporates deep learning for structure-based drug design, enabling the rapid, AI-powered search of Atomwise's proprietary library of more than 3 trillion synthesisable compounds. Insilico Medicine, a clinical-stage drug discovery company, created the first AI-discovered antifibrotic drug and went first-in-human in February 2022. More recently, it has integrated AI chat functionality, Chat GPT, into its PandaOmics platform. This will enable researchers to have natural conversations with the platform, making it easier to navigate complex data and identify potential therapeutic targets and biomarkers. Syngene International, a leading scientific research, development and manufacturing company, has developed \proprietary solutions - Syn.AI™, for AI-based drug discovery and Sarchitect™ for QSAR modeling. These platforms help resolve complex scientific problems across target identification, hit identification, lead optimisation, and translational research. Both platforms are tuned for drug discovery in contrast to the generic tuning capability provided by open-source platforms.

The continuous progress of AI technology is helping accelerate the drug discovery process by enabling researchers to analyse and interpret large amounts of data and identify better drug targets and candidates faster. Consequently, overcoming the challenges faced by pharmaceutical companies. This impact could be a reason behind the increasing number of biotech startups in this industry.

Employing cutting-edge AI technologies not only accelerates the product's time-to-market but impacts many aspects of the pharma value chain too. It improves the quality of the product, strengthens compliance, enhances the overall efficiency of the manufacturing process, makes operations error proof, helps rapid troubleshooting, and is cost-effective

Dr Mahesh Bhalgat, COO, Syngene International