AI in Drug Discovery

Axel Xaverius Ivory
http://orcid.org/0009-0001-7228-8942
Universitas Esa Unggul, Indonesia

Cornelius Adrian Putra
http://orcid.org/0009-0002-2991-4618
Universitas Esa Unggul, Indonesia

Binastya Anggara Sekti
http://orcid.org/0000-0001-5489-4888
Universitas Esa Unggul, Indonesia

ABSTRACT

Artificial Intelligence (AI) is transforming the field of drug discovery by enabling faster, more efficient, and cost-effective processes across all stages of pharmaceutical development. Through machine learning, deep learning, and predictive modeling, AI facilitates virtual screening of chemical compounds, predicts drug-target interactions, and assesses potential toxicity early in the pipeline. These capabilities significantly reduce time and resources traditionally required for laboratory experimentation. Additionally, AI contributes to personalized medicine by analyzing genomic and clinical data to design patient-specific therapies. Despite its advantages, AI-based drug discovery faces challenges such as data bias, lack of transparency in decision-making, and has regulatory uncertainties. This article discusses key AI methodologies, real-world applications, and emerging trends in drug discovery, emphasizing the role of AI as a transformative force in modern biomedicine.

1. INTRODUCTION

Drug discovery is a complex and lengthy process, historically relying on traditional laboratory-based experimental approaches and repeated trials. For decades, this process has been known to be time-consuming, resource-intensive, and often unsuccessful. Many compounds that initially appear promising ultimately fail in preclinical or clinical trials, either due to unexpected toxicity, low efficacy, or unsuitability for scale-up production. The high costs and high risk of failure make drug discovery a major challenge in

DOI: 10.4018/407365

the pharmaceutical and biotechnology industries. Drug discovery aims to identify potential therapeutic compounds capable of modulating the activity of specific biological targets (Bugnon *et al.*, 2024).

However, advances in information and computing technology have brought about significant changes in scientific approaches, including in the pharmaceutical field. One of the most significant innovations of the past two decades has been the advent of Artificial Intelligence (AI). This technology has paved the way for a paradigm shift in drug discovery and development, from a reactive and labor-intensive approach to a proactive, predictive, and big data-driven approach. AI is not only a tool but also serves as a key catalyst in accelerating the process of discovering new pharmaceutical compounds, understanding disease mechanisms, and increasing efficiency and accuracy across various stages of research (Yi and Sen, 2021).

AI works through algorithms designed to mimic the way humans think and learn, but with processing power and speed far beyond human capabilities. Using machine learning, deep learning, and other advanced computing techniques, AI can process large-scale biological, chemical, and clinical data to discover hidden patterns, predict trial outcomes, and even suggest compounds with therapeutic potential. In the context of drug discovery, this means that AI can accelerate the identification of molecular targets, screen thousands of compounds in record time, and even design new molecules that scientists had never previously considered. The integration of machine learning (ML) and artificial intelligence (AI) has transformed traditional processes, creating smarter, more efficient, and adaptable systems (Sekti, 2025b).

One of the most tangible examples of AI applications is in virtual compound screening. This method allows researchers to simulate the interactions between chemical compounds and biological targets in silico (on a computer), without the need for prior physical testing in a laboratory. This process not only accelerates the discovery of drug candidates but also significantly reduces costs. Furthermore, AI can predict the toxicity and potential side effects of a compound early on, thereby reducing the risk of failure in expensive and time-consuming clinical trials (Yi and Sen, 2021).

AI's ability to analyze big data from various sources—such as genomic, proteomic, metabolomic, patient clinical data, electronic medical records, and scientific publications—enables the integration of broad and in-depth knowledge. This is crucial in the era of precision medicine, where therapies are specifically targeted based on a patient's genetic profile and individual characteristics. With the help of AI, this approach becomes more feasible and efficient (Malviya, Malviya and Dhere, 2023).

Beyond scientific and technical aspects, AI also has a significant impact on the economic and business aspects of the pharmaceutical industry. The average cost of bringing a new drug to market can reach more than US$2.5 billion, with development times that can take 10 to 15 years. The application of AI has proven to be able to drastically reduce this time. In some cases, such as during the COVID-19 pandemic, AI has been used to accelerate the identification of potential drugs and vaccine design in a matter of months, something previously nearly impossible to achieve with conventional methods.

Not only large pharmaceutical companies are leveraging AI in research and development, but also biotechnology startups, academic institutions, and government research agencies. Some well-known companies that have developed AI platforms for drug discovery include BenevolentAI, Atomwise, Insilico Medicine, and Exscientia. They use technologies such as deep neural networks, natural language processing (NLP), and generative adversarial networks (GANs) to automatically process and generate new molecules. Collaborations between pharmaceutical companies and technology companies are also becoming increasingly common, signaling a strong synergy between healthcare and the digital world (Malviya, Malviya and Dhere, 2023).