Paradigm Academic Press
Journal of Innovations in Medical Research
ISSN 2788-7022
MAR. 2024 VOL.3, NO.1

Utilizing Artificial Intelligence in the Development of Medicinal Drugs: Practical Applications

Bassam Abdul Rasool Hassan[1] & Ali Haider Mohammed[2]

[1] Department of Pharmacy, Al Rafidain University College, Baghdad, Iraq

[2] School of Pharmacy, Monash University Malaysia, Jalan Lagoon Selatan, Bandar Sunway, Selangor, Malaysia

Correspondence: Bassam Abdul Rasool Hassan, Department of Pharmacy, Al Rafidain University College, Baghdad, Iraq.

doi:10.56397/JIMR/2024.03.04

Abstract

The COVID-19 pandemic has underscored the critical need for innovative drug discovery methods. The journey from conceptualizing a drug to its clinical application is fraught with potential pitfalls, including extensive complexity, significant expenses, and a high risk of failure. Recent years have witnessed remarkable advancements in technologies such as cloud computing, GPUs, and TPUs. These developments, coupled with the surge in medical data availability and the emergence of deep learning, present an unprecedented opportunity to enhance drug discovery processes. By leveraging artificial intelligence (AI) to analyze vast amounts of data-from extensive molecular screening outcomes to individual health records and public health data-the efficiency of the drug discovery pipeline could be significantly improved, minimizing the likelihood of failure.

This paper explores the application of AI in various phases of drug development, including the use of computational strategies for de novo drug design and the prediction of drug properties. We address challenges associated with molecular representation, data acquisition, complexity, and the inconsistencies in labeling across open-source databases and AI-powered tools that support drug discovery efforts. Furthermore, we examine the role of advanced AI techniques, such as graph neural networks, reinforcement learning, generative models, and structure-based methods like molecular docking and dynamics simulations, in enhancing drug discovery and evaluating drug efficacy.

Keywords: artificial intelligence, medicinal drug development, practical applications

1. Introduction

The pharmaceutical sector has seen a marked increase in data digitization efforts in recent years. However, this shift brings about significant challenges in collecting, analyzing, and leveraging vast data sets to tackle complex clinical problems. The adoption of Artificial Intelligence (AI) is largely driven by its capability to handle large-scale data with superior automation techniques. AI encompasses a suite of advanced technologies and frameworks designed to emulate aspects of human intelligence. Importantly, it is not intended to supplant human effort but to augment it. AI systems are built on algorithms that learn from data input, enabling them to independently make decisions aimed at achieving specific objectives. This review delves into how AI applications are continually broadening within the pharmaceutical industry. According to forecasts by the McKinsey Global Institute, the rapid advancement in AI-driven automation is poised to revolutionize societal work paradigms (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz,

Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

1.1 Overview of AI and Its Possible Applications in Pharmaceutical Research

The excitement surrounding the potential of artificial intelligence (AI) to revolutionize medicinal chemistry has grown significantly in recent years. The journey to discover new drugs is an intricate and time-consuming venture, traditionally reliant on resource-intensive practices such as high-throughput screening and empirical research. The integration of AI methodologies, including natural language processing and machine learning (ML), proposes a more efficient and precise approach to analyzing vast datasets. Recent advancements have seen scientists employ deep learning (DL) techniques with notable success in predicting the effectiveness of pharmacological compounds. Furthermore, AI has shown promise in forecasting the toxicity levels of prospective medications. These and similar studies highlight AI's capacity to enhance the speed and efficacy of drug discovery processes (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

Despite the promising advantages of AI, it's important to acknowledge the existing challenges and limitations in applying these technologies to the synthesis of new bioactive molecules. A thorough investigation is essential to fully understand the potential and pitfalls of AI within this field, taking into account the ethical implications. Although hurdles exist, the expectation is that AI will significantly influence the development of innovative treatments and drugs in the foreseeable future. (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021)

1.2 Data Science Is Applied in the Drug Discovery Process

The relentless quest for novel medications is underscored by the emergence of epidemics and pandemics such as COVID-19 and influenza, alongside the widespread incidence of chronic conditions like cancer and cardiovascular diseases. The drug development process is typically a comprehensive multi-phase journey, encompassing target identification and validation, high throughput screening, animal testing, the establishment of safety and efficacy protocols, clinical trials, and finally, securing regulatory approval. On average, bringing a new drug to market demands over 14.6 years and an investment of approximately $2.6 billion. Artificial Intelligence (AI)-based approaches hold promise in streamlining several stages of this intricate process. These include uncovering new therapeutic targets, elucidating disease mechanisms, designing and refining small molecule drugs, and evaluating drug-target interactions. Furthermore, AI techniques can be leveraged to assess pharmacological effectiveness, patient response, and resistance, in addition to identifying and developing predictive biomarkers. This innovation not only has the potential to accelerate the pace of drug discovery but also to make the process more cost-effective and successful (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

1.3 A Look at AI's Function in Measuring Drug Safety and Effectiveness

The application of artificial intelligence (AI) in predicting the safety and efficacy of new pharmaceutical compounds represents a cutting-edge frontier in the field of medicinal chemistry. Traditional methods of assessing a compound's impact on human health are notably rigorous and protracted, characteristic of classical drug discovery processes. These approaches are not only costly and slow but also fraught with unpredictability. AI and related technologies offer a pathway to circumvent these challenges. Through the analysis of vast datasets, AI algorithms can uncover insights and patterns beyond human detection capabilities, potentially accelerating the development of bioactive compounds with minimal adverse effects (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

A noteworthy instance is the deployment of a deep learning (DL) algorithm trained on a dataset comprising known pharmacological molecules and their biological activities. This model subsequently yielded highly accurate predictions concerning the behavior of novel compounds. Moreover, machine learning (ML) has made

significant strides in reducing potential toxicity in new medicinal molecules by training extensively with large datasets of known toxic and non-toxic compounds.

AI also plays a pivotal role in identifying drug-drug interactions, which arise when multiple drugs administered to a patient interact in unforeseen ways, leading to enhanced or diminished effects, or even adverse reactions. AI methodologies excel in navigating through extensive databases of documented drug interactions, identifying patterns that may predict how new drug combinations will interact. Recent advancements include an ML algorithm designed to forecast the outcomes of novel drug combinations effectively (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

In the realm of personalized medicine, AI's capacity to predict drug-drug interactions becomes particularly valuable, facilitating the design of tailored treatment regimens that lower the risk of negative side effects. Personalized medicine aims to customize healthcare, with decisions and treatments tailored to the individual patient, considering their genetic profile and specific responses to medications.

Drawing from the literature and examples cited, it is evident that AI holds the promise to enhance the prediction of toxicity and efficacy in novel therapeutic agents within pharmaceutical research. This advancement could significantly expedite the drug discovery process, paving the way for the development of treatments that are both safer and more effective (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

1.4 Problems and Restrictions with AI for Drug Discovery

Before the potential of artificial intelligence (AI) in drug discovery can be fully realized, it's essential to navigate through several challenges and limitations. Among these, data access stands out as a pivotal hurdle. Effective training of AI methodologies typically requires vast datasets. However, the scarcity of data, alongside issues related to its quality and consistency, can significantly undermine the reliability and accuracy of AI-generated outcomes. Moreover, ethical considerations pose substantial challenges, sparking debates over the fairness and potential biases of AI-driven solutions.

For example, if the data utilized to train AI algorithms is biased or fails to accurately represent the broader population, it could lead to unjust or incorrect predictions. This highlights the critical need for ethical scrutiny and the implementation of measures to ensure fairness in AI's application to the discovery of new pharmaceutical compounds. Addressing these concerns is crucial for harnessing AI's capabilities responsibly and effectively in the quest for novel medical treatments (Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, 2023; Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, 2023; Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia & Rakesh K. Tekade, 2021).

2. Conclusion

Ultimately, artificial intelligence (AI) has the potential to revolutionize the drug discovery process by accelerating development timelines, enhancing accuracy, and boosting overall efficiency. Such advancements could pave the way for the creation of treatments that are not only more effective but also customized to the specific needs of patients. Nonetheless, for AI to truly fulfill its promise in this domain, it's imperative to address its limitations head-on. Tackling ethical concerns, ensuring the fairness of AI applications, and securing access to high-quality data are all essential steps toward the successful integration of AI in drug discovery. By navigating these challenges thoughtfully, we can unlock the full potential of AI to transform medication development for the betterment of patient care and treatment outcomes.

References

Alexandre Blanco-González, Alfonso Cabezón, Alejandro Seco-González, Daniel Conde-Torres, Paula Antelo-Riveiro, Ángel Piñeiro, & Rebeca Garcia-Fandino, (2023). The role of AI in drug discovery: challenges, opportunities, and strategies. *Pharmaceuticals, 16*, 1-11.

Debleena Paulz, Gaurav Sanapz, Snehal Shenoyz, Dnyaneshwar Kalyane, Kiran Kalia and Rakesh K. Tekade, (2021). Artificial intelligence in drug discovery and development. *Drug Discovery Today, 26*(1), 80-95.

Rizwan Qureshi, Muhammad Irfan, Taimoor Muzaffar Gondal, Sheheryar Khan, Jia Wu, Muhammad Usman Hadi, John Heymach, Xiuning Le, Hong Yan & Tanvir Alam, (2023). AI in drug discovery and its clinical relevance. *Heliyon, 9*, 1-23.