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A REVIEW ON DRUG DISCOVERY AND DEVELOPMENT ASSOCIATED WITH ARTIFICIAL INTELLIGENCE

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ABSTRACT
The integration of artificial intelligence (AI) in drug discovery and development has ushered in a new era of innovation and efficiency in the pharmaceutical industry. This review explores the recent progress, challenges, and potential future directions of AI applications in drug research, highlighting its impact on target identification, compound screening, drug design, and clinical trials. Through a comprehensive examination of current literature and case studies, we aim to provide a nuanced perspective on the transformative role AI plays in accelerating drug discovery processes.

INTRODUCTION

The conventional drug discovery and development pipeline is a time-consuming and resource-intensive process. However, with the advent of AI technologies, there has been a paradigm shift in how pharmaceutical research is conducted. AI offers the promise of significantly reducing the time and cost associated with bringing new drugs to market, making it a key player in the quest for more effective and targeted therapeutic interventions. The process of developing new drugs is difficult, costly, time-consuming, and has a high attrition rate.[i] Clinical study drug attritions result in significant resource loss, and nine out of ten drug candidates fail between phase-I clinical trials and regulatory approval at this time.[ii] In drug discovery, difficult chemical search problems are automated by the use of supervised learning on molecules. Finding efficient neural network models with the ability to forecast chemical attributes and possibly automate the search for novel medications or materials is the goal.[iii]

Definition of Drug Discovery: The process of discovering novel drugs to treat illnesses and enhance human health is known as drug discovery. It entails using a variety of computational and experimental techniques to identify and design molecules with the potential to become useful medications.[iv]

Definition of Artificial Intelligence: The study of computer science that focuses on developing intelligent systems that can make decisions and solve complicated issues is known as artificial intelligence (AI). Advanced methods like representation learning and deep learning are frequently used in this process. By offering creative answers to problems that the AI community has historically found challenging, these systems, which seek to mimic human-like intelligence, have the potential to completely transform a number of industries. [v]

A subfield of computer science called artificial intelligence (AI) gives robots the ability to analyze complicated data and operate more productively. AI-focused research has grown significantly, and its application to healthcare services and research is developing at a faster rate. The pros and cons of AI in medical and pharmaceutical research are covered in detail in this paper. Using specific keywords and phrases like "Artificial intelligence," "Pharmaceutical research," "drug discovery," "clinical trial," "disease diagnosis," etc., the literature was gathered from domains like PubMed, Science Direct, and Google Scholar in order to select and review articles published within the last five years. This article explores in great detail the potential applications of AI in disease diagnostics, digital therapy, individualized treatment, drug discovery, and pandemic or epidemic forecasting. The most popular artificial intelligence (AI) technologies are deep learning and neural networks; prospective technologies for clinical trial design are Bayesian nonparametric models; wearable technology and natural language processing are employed for patient identification and clinical trial monitoring. In order to predict the occurrences of COVID-19, Zika, Ebola, and seasonal influenza, deep learning and neural networks were utilized. The scientific community may witness quick and affordable pharmaceutical and healthcare research with the development of AI technology, along with better public services.[vi]

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The COVID-19 pandemic has definitely served as a catalyst for the phenomenal growth of the field of digital health. Both inside and outside of the healthcare industry, the terms "digital health" and "artificial intelligence" are now the most searched. Pharmacists must be active as more AI technologies are being implemented globally in the healthcare industry. Pharmacists may play a major role in integrating technologies that improve patient experience and care because digital health is becoming a significant element of managing long-term diseases, whether it's monitoring symptoms, monitoring adherence, or even the therapy itself. Artificial intelligence has initiated a digital revolution in the pharmaceutical industry as well. It minimizes medical expenses significantly and is used to enhance medication discovery and personalize therapy.[vii]

A number of tools that are based on the networks that make up AI systems' fundamental design have been created. The International Business Machine (IBM) Watson supercomputer (IBM, New York, USA) is one such instrument created with AI technology. It was created to help with the examination of a patient's medical records and their relationship to an extensive database, ultimately leading to the recommendation of cancer treatment plans. Rapid illness detection is another application for this technique. This was shown by the fact that it could identify breast cancer in just 60 seconds.[viii ix]

Drug Discovery through Artificial Intelligence

AI can recognize hit lead compounds and give a faster approval of the sedate target and optimization of the medicate structure plan. Distinctive applications of AI in sedate disclosure are delineated in Figure-1[x xi]. The use of artificial intelligence (AI) in drug discovery is important. This field is mainly driven by neural networks such as recurrent networks and deep neural networks. In recent years, many applications have emerged in vehicle or performance prediction, such as physiochemical and ADMET products, supporting the advantages of this method in relationship between features (QSPR) or multi-model- correlation (QSAR). In de novo design, artificial intelligence guides the creation of new bioactive molecules to achieve desired properties. Many examples have proven the effectiveness of expertise in this field. The combination of simplicity of mixing with synthetic preparation makes this possible, and further exploration in computer aided medicine should be made in the future.[xii]

Compound Screening and Drug design: Virtual screening and in-silico drug design have become integral components of the drug discovery process, thanks to AI. Machine learning models can predict the biological activity of compounds, prioritize lead compounds, and optimize molecular structures for enhanced efficacy. This accelerates the identification of potential drug candidates, reducing the need for extensive laboratory testing.[xiii]

Target identification and validation: AI plays a pivotal role in target identification by analyzing vast datasets to identify potential molecular targets associated with specific diseases. Machine learning algorithms can sift through biological data, including genomics, proteomics, and transcriptomics, to pinpoint novel targets. Moreover, AI assists in target validation by predicting the biological relevance and potential success of targeting specific molecules.[xiv]

Clinical Trials Optimization: AI is streamlining the clinical trial process by improving patient recruitment, optimizing trial design, and enhancing data analysis. Natural language processing and machine learning algorithms analyze vast amounts of clinical and patient data, enabling more efficient and patient-centric trial designs. This leads to quicker recruitment, reduced costs, and improved chances of successful trial outcomes.[xv]

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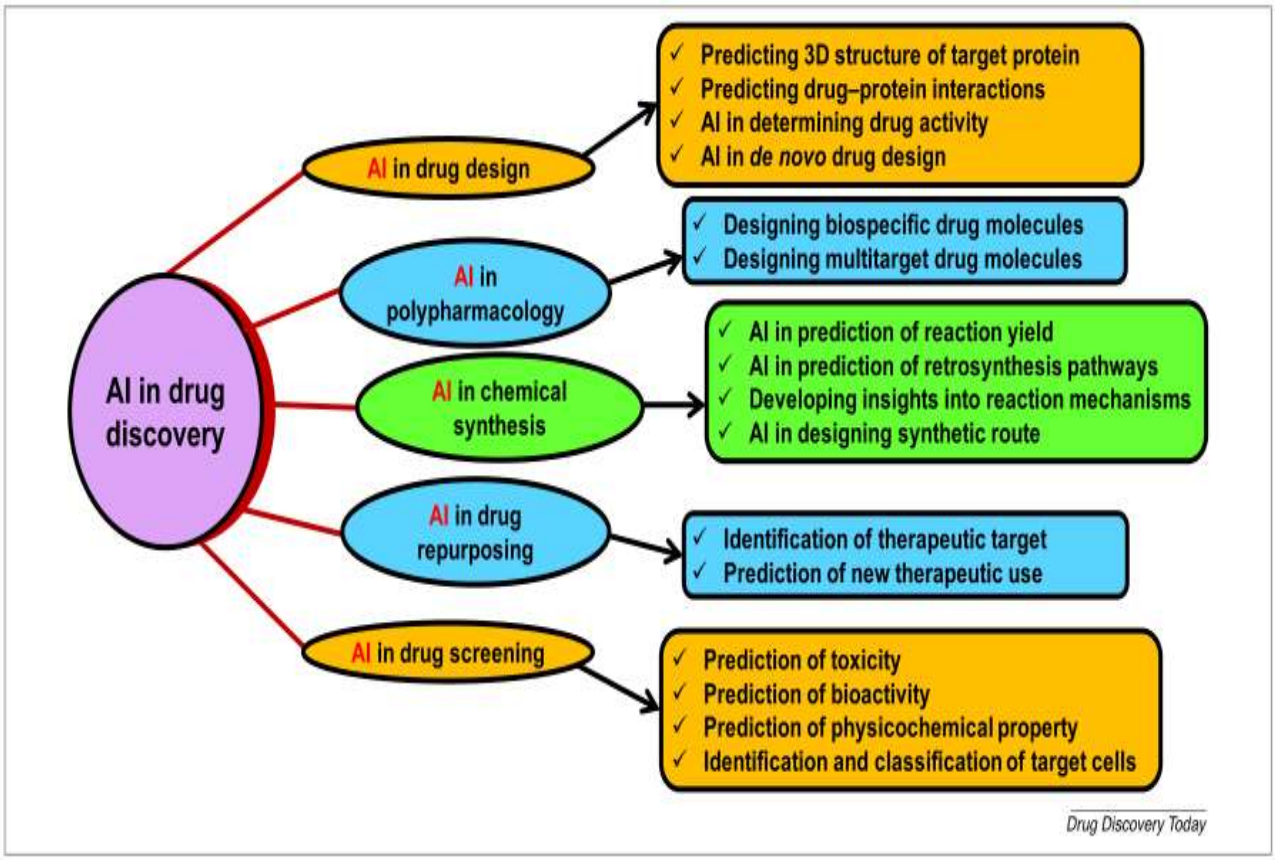

Figure-1

Artificial intelligence involves many processes such as reasoning, knowledge representation, and problem solving, including importan t elements of machine learning (ML). Machine learning uses algorithms that can identify patterns in a more distributed set of data. A s ubfield of machine learning is deep learning (DL), which includes artificial neural networks (ANN). They have an interactive system o f computer networks with "sensors" similar to human biological systems that monitor the transmission of electrical impulses in the hu man brain.[xvi]Artificial neural network consists of a group of nodes. Each node individually takes input and eventually transforms it int o output, algorithms that can be used to solve problems that depend on one or more of them.[xvii] ANNs comes in many forms, including multilayer perceptron (MLP) networks, recurrent neural networks (RNN), and convolutional neural networks (CNN) that use supervised or unsupervised techniques.[xviii xix]

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A summary of AI method domain examples can be seen in Figure 1.

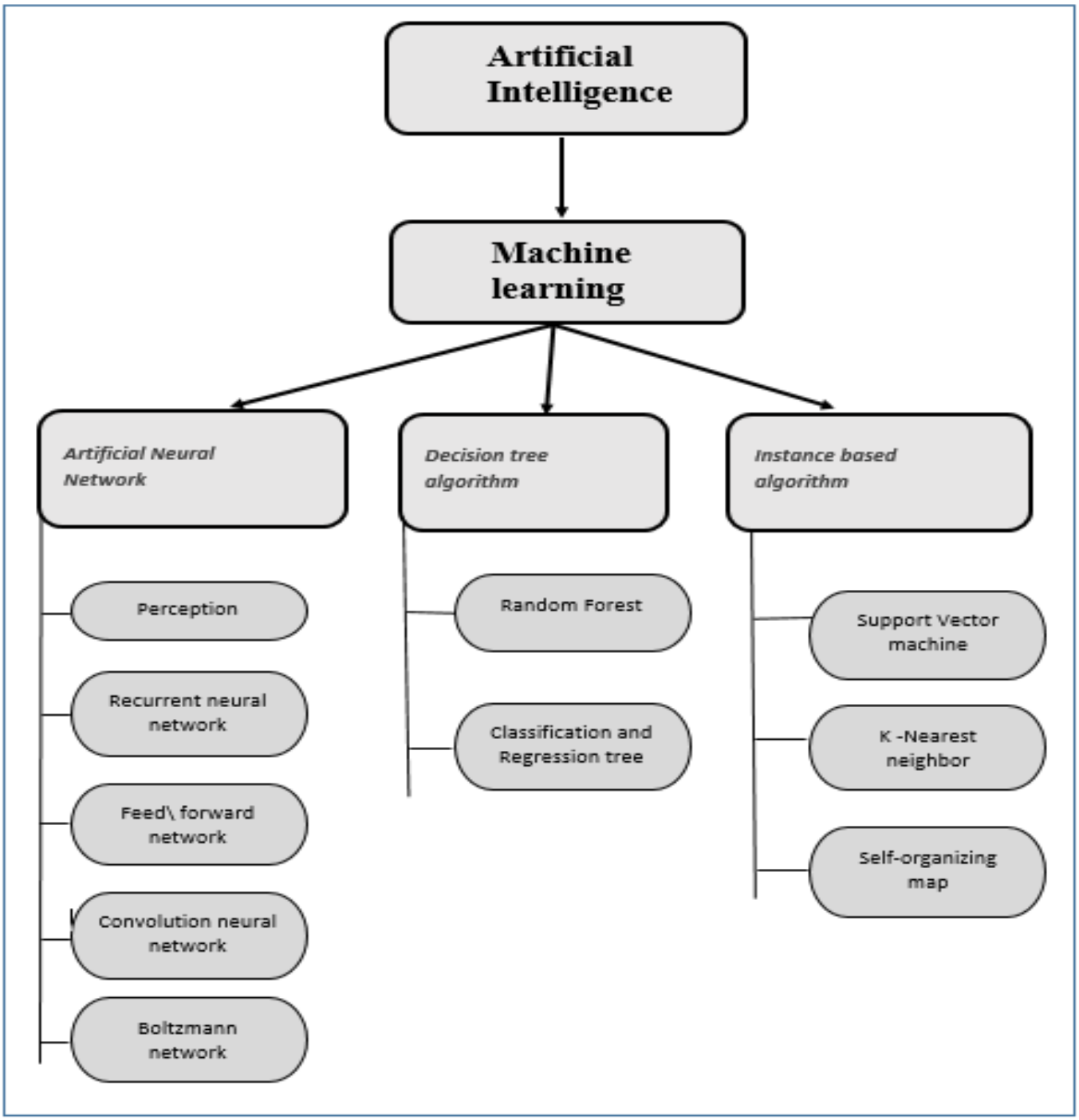

Figure-2

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AI in QSAR\QSPR and Structure based modeling

A computational procedure called Quantitative Structure Activity Relationship (QSAR) is utilized in atomic modeling to estimate a chemical compound's natural movement based on its auxiliary characteristics. It involves the creation and confirmation of scientific models that interface a compound's discernible movement to its chemical structure, advertising experiences for applications such as virtual screening and drug disclousre.[xx] QSAR modeling tools have been used to identify potential drugs users and have been developed into cognitive based QSAR methods such as linear discriminant analysis (LDA), support vector machines (SVM), random forests (RF), and decision trees that can speed up QSAR analysis. Computational models based on the QSAR model can predict large number of compounds or simple physiochemical parameters such as log P or log D. However, these models are still some way off in predicting complex biological properties such as efficacy and side effect of compounds. In addition, QSAR based models face problem such as small training, incorrect experimental data in training and lack of experimental analysis. To overcome these challenges, recently developed artificial intelligence techniques such as deep learning and modeling studies can be used for safety and performance evaluation, quality of drug molecules based on big data and analysis. In 2012, Merck sponsored the QSAR Machine Learning Challenge to evaluate the effectiveness of deep learning (DL) in the drug discovery process in the pharmaceutical industry. Compared with the traditional machine learning (ML) method, the DL model showed significant prediction of 15 Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) datasets of drug candidates.

Artificial intelligence- de novo drug design

De novo design, or creating new molecules from scratch with the desired pharmacological properties, is one large number of chemical space molecules that resemble drugs (roughly 1060-10100).[xxi xxii xxiii] Depending on the material used to guide the de novo design, associations can be ligand-based, structure-based, or a combination of both. Ligand-based approaches can be broadly classified into two groups: (1) rule-based approaches, which assemble molecules from a set of "building blocks" (i.e. reagents or molecular fragments) using a set of construction rules; and (2) rule-free approaches, which do not use explicit construction rules. The topliss technique, for the sequential production of analogs of an active lead molecule to maximize potency, is one of the forefathers of modern rule-based de novo design.[xxiv] In De Novo drug development, we have slowly seen the evolution of legal and non-legal terms over the last few years. Although the latter holds promise for exploring invisible areas of chemical space, it also has limitations, such as restrictions on use. Combining free and custom based approaches (e.g. "hybrid" approaches) can provides practical solutions. Particular attention will be paid to the production process, where additional information such as some functional and genetic conformational space and ligand binding site information can be used.[xxv xxvi xxvii]

Application of AI in Drug Development and Drug Discovery

Considering that artificial intelligence can facilitate the development of appropriate drugs,
it can be predicted that it will be used to support decision making throughout the drug development process, from the laboratory to the hospital, and to choose the best treatment options for patient, including drug therapy and collect medical information designed for use in future drug development.[xxviii xxix]

Computer science's artificial intelligence field think about typical programming as implies of issue understanding. Large scale applications of artificial intelligence can help in settling help care concerns. One vital and effective utilize of artificial intelligence in the creation of master frameworks. A technology based framework known as artificial intelligence (AI) mimics human intelligence by utilizing extends of modern instruments and systems. Artificial intelligence (AI) uses equipment's and program able of pursuing, learning from and making choices on its claim to do certain assignments. This chapter examines the continuous development of its employments within the pharmaceutical industry. The healthcare industry has been managing with a few troublesome issues of late, such rising medicine and therapy cost and society must make a few major alterations in this zone. With AI in pharmaceutical item fabricating, customized drugs with the required dosage, discharge characteristic and other components can be created based on the wants of particular patient. In addition to shortening the time it takes for products to reach the market, utilizing the most recent AI-based technologies will also enhance product quality, increase manufacturing process safety, improve resource efficiency, and highlight the value of automation. In expansion to shortening the time it takes for items to reach the advertise, utilizing the foremost later AI-based innovations will moreover upgrade item quality, increment fabricating handle security, move forward asset effectiveness, and highlight the esteem of computerization.This chapter highlights the importance of artificial intelligence (AI) in the pharmaceutical industry, with a special focus on clinical research, drug development, drug advancement, and drug innovation and its potential for future drug discovery research.

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Challenges and Ethical Considerations

Despite its tremendous potential, the integration of AI in drug discovery comes with challenges, including data quality issues, interpretability of AI models, and ethical considerations. Ensuring transparency, accountability, and ethical use of AI technologies is crucial to maintain public trust and address concerns related to bias and privacy[xxx]

Future Perspective

The future of AI in drug discovery holds exciting possibilities, including the development of AI-driven personalized medicine, drug repurposing, and the emergence of AI-generated novel hypotheses. Collaboration between researchers, clinicians, and technology experts will be essential to harness the full potential of AI in advancing pharmaceutical research and improving patient outcomes[xxxi]

CONCLUSION

In conclusion, the integration of AI in drug discovery and development represents a revolutionary shift in the pharmaceutical landscape. From target identification to clinical trial optimization, AI offers unprecedented opportunities to accelerate the drug development process. As researchers continue to overcome challenges and ethical considerations, the future holds immense promise for AI to reshape the way we discover and develop new medicines, ultimately benefiting patients worldwide. Artificial Intelligence has revolutionized drug discovery and development, offering unprecedented opportunities to transform the pharmaceutical industry. This comprehensive review provides insights into the current state, challenges, and future prospects of AI applications in drug development, emphasizing its potential to accelerate the discovery of innovative therapeutics and improve patient outcomes.

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