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Review Article

How AI Can Revolutionize the Pharmaceutical Industry

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Abstract

The pharmaceutical industry has seen a lot of transformation in the last five years because of technological innovations such as AI. AI-based technologies such as ML and DL are revolutionizing the sector and making processes such as drug discovery, research, dose optimization, therapeutic drug monitoring, drug repurposing, predictive analytics, and clinical trials much easier. Drug development is a complex, time consuming, and labor-intensive process. In some instances, drug development takes up to 10 years and a significant amount of investment. However, AI-based technologies are showing a lot of promise when it comes to simplifying the process and making it less-time consuming. The drug development involves a lot of data. AI-based technologies such as ML shows a lot of promise when it comes to analyzing and managing these large volumes of data making the process more manageable. AI has also simplified the process of identifying therapeutic targets. AI is also being used in drug design to help in making predictions of 3D structure of the target protein and predict drug-protein interactions. Other areas where AI is being used in drug discovery are de novo drug design, optimizing clinical trials, predictive modelling, and precision medicine. Despite the advantages that AI offers in pharma, it has its limitations. For instance, ethical considerations regarding patient data, privacy, and confidentiality remains a key issue. Risk of bias also raises ethical concerns that should be considered. Other limitations are limited skills that make it difficult to optimize AI, financial limitations that make it difficult to invest in AI, and data governance challenges.

Keywords: Artificial intelligence (AI), machine learning (ML), deep learning (DL), drug discovery, clinical trials

Introduction

Artificial intelligence (AI) has brought a lot of transformation in different sectors in the last five years. In the pharmaceutical sector, the usage of AI-based technologies has risen rapidly with statistics indicating different AI-based technologies such as machine learning (ML), data science, deep learning (DL), and advanced analytics are being used increasingly to perform different tasks. Some of the processes that are increasingly employing AI are drug development, drug research, dose optimization, therapeutic drug monitoring, predictive analytics among others.[1,2] AI is revolutionizing the sector with different applications being used to facilitate automation and reduce the overall time it takes to perform different tasks.

One of the areas where AI is making a lot of transformation in the drug discovery process. The drug discovery process is complex, labor intensive, and time consuming. It also involves a lot of data which can be difficult to manage. A1 tools such as data mining and algorithm analysis are making the process of data collection, analysis, and harmonization more effective.[2] The data is also being leveraged to facilitate predictive modeling, drug research, and drug discovery.[2] AI is also improving precision and enlarging the scope of research and development (R&D) in the pharmaceutical sector.[3,4] When it comes to modern pharmacy practice, AI is being used to improve accuracy in the diagnostic process, improve clinical decision through clinical decision support systems, and discover anomalies in areas such as medical imaging.[5] Such innovations demonstrate a lot of potential in the pharmaceutical industry in general. They provide an opportunity to streamline the sector and contribute to greater therapeutic innovations.

The aim of this review is to explore how AI is revolutionizing the pharmacological industry. It explores how AI is being used in different processes including drug discovery, identifying therapeutic agents, and optimizing clinical trials. The paper also explores the limitations of AI and why overcoming these limitations is vital to gain full benefits of AI.

AI in Drug Development and Discovery

The last five years have seen a significant transformation in the drug discovery process because of AI. AI is reducing the time the process takes demonstrating a lot of potential in this area. Drug discovery not an easy process. It is challenging, time consuming, and expensive. The process is also labor-intensive process and involves a lot of trial and error.[6] AI provides an opportunity to make the process much simpler and less time-consuming. Tools such as ML offer an opportunity to accelerate and improve the process. The fact that AI is able to examine and analyze large volumes of datasets within a short time period, makes it possible to identify therapeutic targets easily, screen, model medicines, and forecast the efficacy of drug candidates.[7]

Disease Modelling and Therapeutic Targets Identification

AI can also help to optimize disease modelling and identify therapeutic targets. Disease modelling and identifying therapeutic targets is crucial in drug development.[8] However, despite the significance of this step in the drug development process, it is challenging and uncertain. Target identification involves identifying the right biological entities such as proteins, genes, and RNA that can be modulated by drugs to achieve therapeutic benefits.[8,9] It is important to ensure a target is effective, safe and aligns with the clinical and commercial needs to ensure the drug discovery process is effective. AI offers a lot of opportunities in this process. It provides the advantage because of its ability to analyze large datasets in different areas including genetic and clinical data and its ability to analyze complex biological networks.[4] By analyzing large datasets, AI offers an opportunity to identify potential therapeutic targets through deep learning models and AI algorithms.[8] Al algorithms have the potential to reveal patterns and relationships within the data increasing accuracy and understanding of disease patterns. AI also has the potential to generate synthetic data which can help to identify therapeutic targets.[8] Just like the name suggests, synthetic data is artificial but mimics real-world data patterns. The data can be used to simulate different biological scenarios with the help of AI algorithms.[8] Synthetic data can be a valuable asset where experimental data is scarce. For target identification, this data can be used to train AI models making it a valuable asset in research.

AI in Drug Design

AI can also be used in drug design. It can help to predict the 3D structure of target protein, drug-protein interactions, and to determine drug activity. [10] Predicting the correct target protein structure is vital when it comes to developing a drug module. Different proteins account for different diseases. As a result, predicting the structure correctly for the drug module is vital to ensure appropriate targeting of the disease is done.[11] AI has proved instrumental in this role because the design aligns with the chemical environment of the target protein site which makes predicting the effect of a compound on the target possible.

Using AI to Predict Drug-Protein Interactions

AI in can also be used to predict drug-protein interactions. These interactions are vital in the drug development process. Predicting how drugs interact with a protein is important to understand its efficacy and effectiveness. It also enables the repurposing of drugs and prevents interaction with multiple targets hence reducing expenditures associated with the process and preventing adverse effects.[10] Different AI tools play a critical role when it comes to making correct predictions. One of these tools is AlphaFold, which is an AI tool that is based on deep neural networks (DNNs). The tool helps to predict protein interactions by analyzing the distance between the adjacent amino acids and the corresponding angles of the peptide bonds.[10] The tool correctly predicted 25 out of 43 structures which means that it has a high accuracy rate.[10,12]

AI in De Novo Drug Design

Another area where AI can play a critical role is in de novo drug design which is a process of developing novel molecular structures from scratch.[13] The process is done from atomic building blocks that have no previous relationships. The process is complex process. Conventional methods of drug design are based on evaluating the existing substances for possible activity against a target.[14] These conventional methods are mainly structure-based and ligand-based designs. These designs depend on the properties of the active site of a biological target or the known active binders.[13] However, with AI and tools such as ML this is changing. Machine learning provides computational intelligence which makes it possible to create customized and potent medication candidates.[15] ML makes it possible to design molecules that have desired features because of its ability to make predictions, analyze data sets, and spot trends ML also makes it possible to use data to make suggestions of new molecule structures that interact well with target proteins. Another role of ML is to create viable and physiologically active compounds which can be challenging during drug discovery.

Using AI to Optimize Clinical Trials

Another important role of AI is optimizing clinical trials. Clinical trials are important in developing new therapeutic agents because they are used to determine the safety and efficacy of the developed drugs for human subjects and whether or not they have any side effects.[10] Despite the significance of clinical trials, they are expensive, time-consuming and in some cases do not produce the desired results. In some instances, clinical trials take as long as 15 years.[16] Despite the effort and financial investment dedicated to this process, only one out of ten molecules that join these trials are cleared successfully by the Federal Drug Administration (FDA).[17] Different factors contribute to high failure rates experienced during clinical trials. They include design flaws characterized by inadequate sample sizes, inappropriate patient selection, safety issues, inadequate clinical efficacy, toxicity, and poor drug-like properties.[18,19]

The entrance of AI in the pharmacological sector offers a lot of promise for clinical trials. Due to the large amount of medical data available, failures attributed to clinical trials can reduced significantly. ML offers the opportunity to transform clinical trials because it provides data-driven insights that can improve the trial design significantly.[15,20] Data-driven insights can also improve patient recruitment, design, and decision-making reducing the failure rate of these trials significantly. Additionally, ML algorithms can be used to find variables such as patient characteristics, dosage schedules, and biomarkers that can lead to positive outcomes. This can be done by examining past trial data. Using data to find variables that are likely to lead to positive outcomes can increase efficacy and lead to better targeted investigations which can save time and costs associated with clinical trials. Machine learning computational tools can also aid in the computation-aided drug design process.[21] Recruiting patients for clinical trials remains a major challenge because of high dropout rates and challenge of finding suitable volunteers.[15] Challenges in finding the right patients for the trial slow down the trial development significantly and can slow down the process. Deep learning models can aid in this process.[22] Because of its data insight, they can be able to forecast the eligibility of patients in clinical trials.

AI in Predictive Modeling and Real-Time Data Monitoring

Other advantages of ML in clinical data are providing an opportunity for real-time data monitoring and also predictive modeling. Real-time monitoring is significant in clinical trials. Researchers use it to identify anomalies, if there are changes in patient behavior, indications of adverse events, and whether or not treatment is effective. [10] It can be easy to miss such information when using traditional monitoring of patients.[10] Real-time monitoring is instrumental because it enhances patient safety and provides data insights that can be used to make trial modifications.[16] AI-based technologies such as machine learning can be used to perform predictive modelling.[23] Machine learning plays an instrumental role in making forecasts of patient reactions to medication. This data is based on patient traits, genetic profiles, and biomarker information. Forecasting patient reactions is vital in optimizing dosage regimens. It also helps to decrease the probability of patients having adverse reactions and improves the overall outcome of the clinical trial.

AI in Drug Repurposing

AI-based technologies are also used in drug repurposing and in predicting drug toxicity. Drug repurposing is an important aspect of the drug discovery process because it is more cost-effective. It is used to identify novel medications. Drug repurposing plays an instrumental role in helping to identify new therapeutical applications for medications that are approved for other purposes.[15] AI-based applications such as machine learning can help in the process because of their ability to analyze large sets of biomedical data and carry out computational analysis which are crucial for new drug discoveries.[4] AI can help to accelerate the process and reduces the associated costs. When it comes to predicting drug toxicity, Al can improve and make it more efficient. ML algorithms can be trained on toxicology databases to anticipate the harmful effects of the drugs and to identify any structural properties that are hazardous.[4] This can improve the safety of the whole process.

The success of AI in drug discovery cannot be denied. The last five years have seen significant discoveries in this area demonstrating its potential. For instance, Exscientia announced the first AI-designed drug molecule to enter human clinical trials in early 2020.[24] The molecule was designed for Sumitomo Pharma Co., Ltd. for obsessive-compulsive disorder and took an average of 12 months. Since this first historical development, Exscientia has created an additional six molecules all designed through generative AI.[25] Other important milestones in the use of AI in drug discovery have also been made by AbSci and Insilico Medicine.[24]

The Use of AI in Pharmacological Research

An additional area where AI has contributed significantly is in pharmacological research. Research is an instrumental part of developing new therapeutic agents and which explains why research and development is vital. Pharmaceutical research requires a lot of insights and knowledge. These insights and knowledge are mainly obtained from biomedical data. The last decade has seen a significant increase in biomedical data as interest in research grows significantly. Entrants of new experimental techniques have also seen a lot of data being collected to aid in pharmaceutical research. Using biomedical data efficiently for research is a challenging process because in most cases it is noisy data.[26] AI plays a key role in managing this data and making it meaningful for research purposes.[27] AI accelerates the process of analyzing this data and reduces the likelihood of errors.[28]

The ability of A to AI to extract patterns from complex data sets is what makes it vital in pharmaceutical research. These datasets are then used to make accurate predictions and informed decisions for research.[29] DL is one of the AI-based applications that has contributed significantly to data analysis. Deep learning models have multiple learnable stages which makes them instrumental in tackling complex data.[30] DL can also be used for unsupervised learning making which makes it vital in interpreting unlabeled data. The ability of AI to interpret unlabeled data makes it instrumental in research because it significantly improves the overall research process. AI is also instrumental in image analysis, facilitating biomarker identification, and optimizing drug formulation. The ability of AI techniques to perform these roles has been instrumental in overcoming the challenges experienced during the drug development process.

AI in Dose Optimization and Therapeutic Drug Monitoring

In addition to advancements in pharmacology, AI has been instrumental in the precision or personalized medicine more so dose optimization and drug monitoring.[31] Dose optimization is instrumental in achieving positive patient outcomes. According to Singh et al., it takes into account patient characteristics such as genetics, age, comorbidities, and clinical information to customize treatment strategies based on these characteristics.[28] Dose optimization increases the chances of optimal patient outcomes because of customization based on patient needs. Advancements in AI have been crucial in dosage optimization. The ability of AI algorithms to store and analyze large datasets, patient clinical information and biomarkers has led to significant transformation in dose optimization with AI being able to determine the optimal drug dosages based on patient needs. One AI-powered platform that has been crucial in personalized medicine is CURATE.AI. CURATE.AI helps with dose recommendations. It does this by mapping the relationship between input (drugs) vs. output for an individual based on their personal data.[31] Based on the predictions, the platform makes recommendations for the intensity of the intervention that can lead to better results. CURATE.AI also monitors the patient's disease progressional over time and makes recommendations on additional drugs, dose changes, and other interventions that are more effective.[32] The platform has been used for dose optimization for patients who have multiple myeloma and metastatic prostate cancer.

Integrating AI in Modern Pharmacy Practice

AI-based applications are not only instrumental in pharmaceutical research but can also be integrated in modern pharmacy practice. AI-based applications can be used to personalize and provide and real-time data to both patients and providers which can help to improve the process of care significantly. One of the areas where can be used in modern pharmacy practice is to increase medication adherence.[33] Integrating AI-based applications with medication reminders can increase patient adherence to medications and reduce the likelihood of missing their doses by providing patients with timely reminders. AI-based tools can also be used to aid in patient communication. For instance, an AI-powered conversational agent has the ability to interpret the requests of patients and respond to their questions in a timely manner.[34] Providing such support to patients leads to better engagement with care and improves satisfaction.

An additional area where AI-based applications can be used is to monitor drug interactions in patients and identify adverse reactions. Although adverse reactions are rare, they still occur and cause patients' untold pain and suffering. These reactions affect patient safety and contribute to high cost of care in bid to address them. Integrating AI-based applications in pharmacy practice can help to minimize the likelihood of these adverse reactions and lead to better patient outcomes. AI can perform different tasks such as monitoring patients, and providing alerts when and if these reactions occur.[34] Other applications of AI in pharmacy practice are managing chronic disease, providing patient education, helping to make dosage adjustments, and medication reconciliations.[35] Incorporating AI in modern pharmacy practice can improve clinical decision-making significantly. It can also enhance accuracy in drug dispensing leading to enhanced patient safety.

Limitations of AI in Pharmacology

Despite the advantages of AI in pharmacology, some challenges are evident. For instance, insufficient skillsets to operate AI-based platforms and algorithms limits its potential in pharma.[36] Data governance is also a significant challenge when it comes to the use of AI in pharma. The drug discovery and development process involves the use of a lot of data. Integrating this data can be a challenge.[37] Lack of investment in AI and limited finances by small organizations are additional challenges that make it difficult to capitalize on AI in the drug development process.

Another area of concern when it comes to using AI in pharmacology is ethical issues. AI-based approaches raise concerns over data safety and security. Privacy issues concerning patient data and usage are likely to emerge.[38,39] AI techniques rely heavily on data. In most cases, this data is sensitive and personal. The risk of access to this data by unauthorized personnel is often evident. Protecting the privacy and integrity of this data should be a top concern for those involved. Adhering to protection laws and regulations is paramount. Measures such as ensuring data anonymity and having strong encryption methods can help.

An additional ethical concern about using AI algorithms and techniques in pharmacological research and drug discovery process is the potential for bias which may lead to unfairness.[40] The potential for bias emerges from the fact that data used to train AI algorithms can be unrepresentative increasing the risk of making inaccurate predictions.[39] Having unrepresentative data can lead to unfair treatment of certain populations bringing about the question of justice and equality. ML models can also reinforce biases that are found in training data leading to discriminating results. Biased algorithms can negatively affect the drug discovery process because they can increase the risk of having inaccurate diagnoses.[15]

Overcoming these challenges presents a lot of opportunities for the pharmacology industry to optimize the drug discovery process through AI. AI can save the industry billions of dollars and time used in the drug development process.[41] Therefore, there is a need for industry stakeholders to find measures to address the challenges identified to optimize AI use in pharmacology.

Conclusion

The significance of AI in pharmacology cannot be denied. Research has demonstrated that different areas of AI such as ML, data science, DL, and advanced analytics are being used in different stages of drug development and discovery. Some of the areas where AI is being used are drug design, disease modelling and therapeutic agents' identification, de novo drug design, predicting drug-protein interactions, optimizing clinical trials, and drug repurposing. In all these areas, AI has demonstrated significant potential. For instance, data mining and algorithm analysis are making it easier to collect and analyze large biomedical data sets which is leading to greater efficiency. ML has also led to greater precision and wider scope in R&D. Other uses of AI technologies across the industry are facilitating automation, providing greater insights into data, and improving decision-making. AI has also been instrumental in precision medicine by helping in dose optimization and drug monitoring. This has been possible because AI-based applications are able to analyze patient data such as clinical information and other biomarkers which makes it possible to determine optimal drug dosages for patients based on their needs and make recommendations. However, despite these advantages, it is important to recognize the challenges presented by AI. Some of these challenges are insufficient skills to operate AI-based platforms and algorithms, challenges with data governance, lack of investment in AI due to limited finances, and ethical issues. Addressing these challenges can lead to a lot of opportunities for the pharmacology industry to optimize the drug discovery process through AI-based applications.

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