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Review Paper

Review On AI Drug Discovery or Development

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ABSTRACT

Artificial Intelligence (AI) has emerged as a transformative technology in the pharmaceutical industry, particularly in medicinal chemistry and drug discovery. Traditional drug development is a complex, time-consuming, and costly process with a low success rate, often requiring extensive experimentation and significant financial investment. AI techniques, including Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP), and Neural Networks (NN), offer innovative solutions to overcome these challenges by enabling efficient analysis of large datasets, accelerating target identification, optimizing lead compounds, and predicting drug efficacy and toxicity. AI-driven tools such as virtual screening, Quantitative Structure–Activity Relationship (QSAR) modeling, and predictive analytics have significantly improved the speed and accuracy of drug discovery processes. Furthermore, AI applications extend beyond drug discovery to pharmaceutical manufacturing, clinical trial design, market prediction, and product cost analysis, enhancing operational efficiency and decision-making. Generative AI technologies, including Generative Adversarial Networks (GANs), are also revolutionizing data generation, medical imaging, and personalized medicine. Despite its advantages, the adoption of AI in the pharmaceutical sector faces challenges such as data quality limitations, ethical concerns, interpretability issues, and regulatory uncertainties. Nevertheless, the integration of AI with traditional experimental methods holds great promise for improving drug development efficiency, reducing costs, and delivering safer and more effective therapies to patients.

INTRODUCTION

The use of artificial intelligence (AI) in medicinal chemistry has acquire significant attention in recent years as a possible way of revolutionizing

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the pharmaceutical industry [1]. In drug discovery the process of identifying and developing new medicine, is a complex and time-consuming attempt that depends on labor-intensive techniques, such as trial-and-error experimentation and highthroughput screening. However, AI techniques such as machine learning (ML) and natural language processing offer the possibility of speeding up and improve this process by enabling more efficient and accurate analysis of large amounts of data [2]. Developing a new drug generally costs over $2.5 billion on average and can take very long time to complete [3]. Moreover, only a small fraction of drug candidates that enter clinical trials ultimately receive regulatory approval [4]. Despite the efforts, only 2.01% of drug development projects ultimately result in a successful marketable drug [5].

Traditional drug discovery and development are characterized by severe restriction that contribute to their high costs, extended timelines, and frequent failures. These restrictions include the back breaking and time-consuming process of identifying promising drug targets; the resource-intensive nature of high-throughput screening for lead compounds; repetitive and expensive optimization of lead compounds to increase efficacy, selectivity, and safety; and the challenges associated with designing and conducting efficient clinical trials, including patient recruitment, data collection, and analysis. These restrictions significantly affect the efficiency and success rate of drug development, hindering the timely delivery of innovative therapies to patients [6].AI tools are being used to solve big problems in finding new medicines, helping doctors take better care of patients, and making healthcare systems work more efficiently [7,8].AI refers to a wide assembling of technologies that allow and help machines to replicate human intelligence, including learning, reasoning, and decision-making [9]. ML, a branch of AI, enables systems to learn from data and enhances their performance on specific tasks through experience, without the need for explicit programming [10,11]. DL is a specialized type of ML that uses Artificial Neural Networks (ANN) with multiple layers ("deep" networks) to identify complex patterns and derive meaningful insights from data [12,13]. Neural networks (NN), inspired by the human brain, are interconnected networks of nodes that process information in a layered fashion, enabling them to learn and make predictions [14,15].AI approaches offer distinct advantages for drug discovery. ML algorithms, such as support vector machines (SVMs) and random forests, perform tasks such as drug-target identification which helps to identify the target and virtual screening [16, 17]. DL, particularly with convolutional neural networks (CNNs), involves in tasks such as de novo drug design, predicting drug-protein interactions, and analyzing medical images [18, 19]. NN, as foundational components of both ML and DL, are strongly used across various stages of drug discovery, including drug toxicity prediction and disease progression modelling [20].The successful use of deep learning (DL) to predict the efficacy of drug compounds with high accuracy has been described recently by the authors of [21]. AI-based methods have also been able to predict the toxicity of drug candidates [22].E-VAI is an analytical and decision-making AI platform developed by Eularis, which uses ML algorithms along with an easy-to-use user interface to create analytical roadmaps based on competitors, key stakeholders, and currently held market share to predict key drivers in sales of pharmaceuticals [23].

❖ AI IN DRUG DRUG DISCOVERY:

AI is used in drug discovery for design of novel compounds which have specific properties and activities. In old time the drug discovery methods

often rely on the identification and modification of existing compounds, which can be a slow and labor-intensive process. On the other hand Ai based approaches, can enable the fast and efficient design of novel compounds with desirable properties and activities and it is not labour intensive. For example, a deep learning (DL) algorithm has recently been trained on a dataset of known drug compounds to propose new therapeutic molecules [24] with desirable characteristics such as solubility and activity, demonstrating the potential of these methods for the fast and efficient design of new drug candidates.

Recently, DeepMind has made a important contribution to the field of AI research with the development of AlphaFold, it is an revolutionary software platform for advancing our understanding of biology [25]The application of Artificial Intelligence(Ai) across the crucial phases of drug discovery specifically target identification, validation, and lead optimization is detailed below:

1. Target identification and validation:

AI algorithms like ML and DL can identify novel targets more effectively than traditional methods by integrating genomics, proteomics, and other sources [26]For example, AI can understand and check genomic data to identify genetic variations associated with diseases and identify genes and their encoded proteins as potential targets [27]. Similarly, AI can also analyze proteomic data, such as protein structures and interactions, to identify proteins involved in disease pathways and assess their drug ability [28, 29]. Moreover, AI can integrate multiple data sources such as DrugBank [30], PubChem [31], Antibiotic Combination Database (ACDB) [32],etc.ML algorithms, such as DL and NLP, are important for analyzing complex datasets and identifying patterns and relationships between molecules that may not be easily visible to human researchers [33].These models can process complex datasets, such as gene expression profiles, single-nucleotide polymorphisms (SNPs), and protein-protein interaction networks, to untangle patterns and relationships that traditional analyzing methods might miss. For instance, supervised learning algorithms such as SVMs and random forests can be trained on labelled gene expression and disease status datasets to predict disease risk and identify genes linked to disease susceptibility [34,35].

2. Drug screening and lead discovery:

AI-powered virtual screening and in silico approaches have revolutionized the identification of potential lead compounds for drug discovery. These methods utilize computational techniques to rapidly evaluate vast chemical libraries, significantly increase the speed of the process and reducing costs compared with traditional screening methods [36,37].

ML algorithms are essential for these methods used for drug screening and lead discovery. They can be used to create quantitative structure–activity relationship (QSAR) models, these models are used to predict the biological activity of compounds based on their chemical structures [38]. Then these models can be used to screen large chemical libraries and prioritize compounds with the highest probability of binding to the target of interest [39]. These AI-driven approaches have the ability to accelerate the identification of promising lead compounds and ultimately improve the success rate of drug development [40].Quantitative structure-activity relationship (QSAR) is computer based model that can quickly predict large numbers of compounds or simple physicochemical parameters, such as log P or log D. However, these models are used for the predictions of complex biological properties, such as the efficacy and adverse effects of compounds. In addition, QSAR-based models also face

problems such as small training sets, experimental data error in training sets, and lack of experimental validations. To overcome these challenges, recently developed AI approaches, such as DL and relevant modeling studies, can be implemented for safety and efficacy evaluations of drug molecules based on big data modeling and analysis[41,42].

3.Drug optimization and design:

AI-driven techniques are revolutionizing drug development by optimizing critical properties, such as solubility, stability, and bioavailability [43]. ML algorithms can analyze large number of datasets of chemical structures and their properties to predict crucial parameters with high accuracy [44]. For example, In QSAR predictions, approximately 1000–5000 data points were used for water solubility predictions [45], whereas DL models can be used to predict drug stability under various conditions [46]. For the protein function prediction task, researchers can leverage two open databases -the UniProt Consortium [47] and the Protein Data Bank (PDB)-to gather protein sequence data from various species [48]. This data can then be used to train prediction models through processes like batch downloading, data cleaning, and pre-processing [49]. These predictive models enable researchers to rapidly identify and optimize drug candidates with improved physicochemical properties, thereby increasing their chances of successful clinical translation [50]

❖ AI TECHNIQUES IN DRUG DISCOVERY:

Some ai techniques which are used in drug discovery are machine learning algorithm (ML), deep learning (DL),natural language processing which is used in identification of novel candidates, molecular printing,etc. From all of these DL and ML technique is generally used. In MLusing supervised and unsupervised learning and DL is used for drug design.

Machine learning Ml algorithm:-Based on the examination of a large amount of information, ML algorithms can easily identify patterns and trends that may not be visible to human researchers. This can enable the proposal of new bioactive compounds with minimum side effects in a much faster process than when using classical protocols. For example, a DL algorithm has recently been trained using a dataset of known drug compounds, with their equivalent biological activity [51]. The algorithm was then able to predict the activity of novel compounds with high accuracy in the result . Important contributions to prevent the toxicity of potential drug compounds, employing intensive training using large databases of known toxic and non-toxic compounds for ML, have also been published [52].

Another important application of AI in drug discovery is the identification of drug–drug interactions that that happens when several drugs are combined for the same or different diseases in the same patient, resulting in change effects or adverse reactions. This issue can be identified by AI-based approaches and by analyzing large datasets of drug which have known interaction and recognizing the patterns and trends. This has been recently addressed by an ML algorithm used to accurately predict the interactions of novel drug pairs [53]. The role of AI to identify possible drug-drug interactions in the context of personalized medicine is also relevant, enabling the development of custom-made treatment plans that minimize the risk of adverse reactions. Personalized medicine aims to tailor treatment to the individual characteristics of each patient, including their genetic profile and response to medications. The previous examples from the literature demonstrate that the use of AI in pharmaceutical research offers the ability to improve the prediction of the efficacy and toxicity of potential drug compounds. This can enable the development of more effective and safer

medications and accelerate the drug discovery process.

Deep learning DL:-DL approaches have shown improved performance compared with ML because they apply network-based methods that do not depend on the availability of the 3D protein structure [54]. DeepDTA, PADME, WideDTA, and DeepAffinity are some DL methods used to measure DTBA. DeepDTA accepts drug data in the form of SMILES, and the amino acid sequence is entered for protein input data and for the 1D representation of the drug structure [55].Deep learning is transforming structure-activity relationship (SAR) modeling, a vital component of drug discovery. Unlike traditional methods that rely on manual feature selection, DL models autonomously extract complex patterns from molecular data, improving prediction accuracy and reliability. For instance, Convolutional Neural Networks (CNNs) can identify subtle structural details to predict key properties like binding affinity, solubility, and metabolic stability [56]. Deep neural networks (DNNs), mainly CNNs and RNNs, are very highly effective tools in drug design. CNNs excel at processing image-like data such as molecular structures represented as 2D or 3D point clouds. They can effectively learn complex patterns within molecular structures, enabling accurate predictions of protein–ligand binding affinities and other crucial properties [57].

✞ AI IN CLINICAL TRAILS :

Testing new medicines in people is a long and expensive process. It usually takes about 6 to 7 years of work and costs a massive amount of money to prove that a drug is both safe to use and actually works for a specific illness.Even though companies spend all that time and money, most of these projects don't actually make it. In fact, only about 1 out of every 10 drugs that start these trials ends up being approved for sale. This means 90% of the time, the drugs fail. For the pharmaceutical industry, this is a huge problem because they lose all the money and effort they put into the nine drugs that didn't work[58].These failures can result from inappropriate patient selection, shortage of technical requirements, and poor infrastructure. However, with the vast digital medical data available, these failures can be reduced with the implementation of AI[58]. AI, such as predictive ML and other techniques, help in the early prediction of lead molecules that would pass clinical trials with consideration of the selected patient population [59].

The company named as AiCure created a specialized mobile app which is designed to help people who are living with schizophrenia stay on track with their treatment during a Phase II clinical trial.

The software worked by monitoring patients to make sure they were taking their prescribed doses of medicine exactly when they were supposed to. This technology made a huge difference in the study's results. By providing this digital monitoring, the app helped increase patient adherence- basically how well people stick to their medical plan-by a significant 25%. Because the participants were much more consistent with their medicine than they might have been otherwise, the researchers were able to collect high-quality data and successfully bring the entire clinical trial to a finish [60].

✞ AI MARKET PREDICTION AND ANALYSIS :

Ai plays an important role in the marketing prediction and analysis for example -Many businesses to business (B2B) companies have launched self-service technologies that allow countless browsing of health care products, easily found by giving its details such as name of medicine or any reference, place orders, and track their shipping. Pharmaceutical companies are also

introducing their online applications such as 1 mg, Medline, Netmeds, and Ask Apollo, to fulfill the needs of the patients [61]. Prediction of the market is also important for many pharmaceutical distributor companies, which can use AI in the field, like 'Business intelligent Smart Sales Prediction Analysis', which uses a combination of time series forecasting and real-time application. This helps pharmaceutical companies to predict the sale of products in advance to prevent costs of extra stock or prevent customer loss because of shortages and fulfill customer demand[62].

Modern AI software is changing how medical products are marketed by reaching both patients and doctors at the same time. These smart systems use data to show personalized ads to the right people at the right moment. For patients, the AI shares helpful health information that catches their interest. For doctors, it highlights new treatments or medical tools that could help their patients. The best part is how simple it is one quick click on the ad takes the user directly to the product's website from which the user can easily search, surf or buy medicines. This makes it easy for everyone to find the clinical details or product info they need instantly, without having to search for it themselves[63].These tools use AI to "read" the words customers type into search bars or chat boxes. By understanding those keywords, the system can spot patterns in how people talk or search. It then uses that information to figure out if someone is just looking around for fun or if they are actually serious about buying a product soon[64,65].

✞ AI IN PRODUCT COST :

After the manufacturing of new product is done by pharmaceutical companies , they need to decide how much to charge for it. To do this, they look at two main things: how much money they spent developing the new product and what the current market looks like. The most important part of using Artificial Intelligence (AI) for this task is its ability to "think" like a human expert, Ai can think like human expert and give the wanted information after giving some commands to it. Instead of just doing basic math, the AI mimics the way a specialist evaluates the different factors that influence a product's price once it is ready to be sold [66].

Factors, such as expenditure during research and development of the drug, strict price regulatory schemes in the concerned country, length of the exclusivity period, market share of the innovated drug after a year before are patent expiry, price of the reference product, and price-fixing policies determine the price of branded and generic drugs [67].In simple terms, machine learning helps businesses set the right prices by analyzing huge amounts of data, like manufacturing costs, market demand, and what competitors are charging. By studying all this data, the software creates smart rules (algorithms) that can predict the best price to set. Software uses this information to create smart formulas that predict the best price for a product.A great example is In competitor, a tool launched by Intelligence Node (founded in 2012). This AI platform tracks and analyzes competitor prices in real-time, this helps brands and retailers stay updated on the market so they can adjust their own prices and stay ahead of the competition.[68]

✞ GENERATIVE AI:-

Generative AI like ChatGPT offers significant promise for healthcare and pharmacy by streamlining tasks such as prescription reviews, drug interaction checks, and adverse event monitoring. While these tools can improve clinical efficiency and patient care,. However, their application in pharmacy education remains underexplored, with limited research on implementation challenges, underscoring the need for further investigation [69].

Generative AI is revolutionizing the medical world by doing more than just helping doctors with basic clinical practices; it has the incredible ability to take massive, complicated datasets and convert them into "predictive models" that help researchers guess the possibilities of what might happen to patients in the future. The heart of this technology is a specific framework called a Generative Adversarial Network, or GAN.GANs stand out as a powerful DL framework made up of two competing neural networks-a generator that creates synthetic data and a discriminator that evaluates its authenticity. Through repetative adversarial training, the generator refines its outputs to produce highly realistic data, enabling applications in medical imaging, super-resolution, and data augmentation [70].One example of this technology in action is the Super-Resolution Generative Adversarial Network, often shortened to SRGAN. This is a specific type of AI has shown impressive results when it comes to taking blurry or low-quality images and digitally convert and enhance them to look sharp and detailed. For example, in the medical world, it helps doctors get a clearer look at diagnostic scans, and in the world of security, it allows
surveillance teams to zoom in on grainy video footage to see important evidence more clearly [71].Moving forward, realizing the full power of Large Language Model (LLM) driven biotechnology will require establishing strict performance benchmarks, upgrade model transparency, and encouraging deeper collaboration between computational and life science communities. This technological merging promises to fundamentally reshape research methodologies and industrial processes across the biological sciences [72].

✞ CHALLENGES AND LIMITATIONS OF AI IN DRUG DISCOVERY:-

Other than the potential benefits of AI in drug discovery, there are several challenges and limitations that must not be neglected. One of the key challenges is the availability of suitable data [73]. AI-based approaches typically require a large volume of information for training purposes[74]. In many cases, the amount of data that is easily understandable may be limited, or the data may be of low quality or inconsistent, which can affect the accuracy and reliability of the results [75]. Another challenge is presented by ethical considerations[76]. since AI-based approaches may raise concerns about fairness and bias [77]. For example, if the data used to train an ML algorithm are biased or unrepresentative, the resulting predictions may be inaccurate or unfair [78]. Ensuring the ethical and fair use of AI for the development of new therapeutic compounds is an important consideration that must be addressed [79].

Current AI-based approaches are not a substitute for traditional experimental methods, and traditional methods cannot replace the expertise and experience of human researchers.[80,81]. AI can only provide predictions based on the data available, and the results must then be checked and interpreted by human researchers [82]. However, the integration of AI with traditional experimental methods can also enhance the drug discovery process [83].Interpretability and transparency is also a significant challenge to the widespread adoption of AI systems is their inherent complexity and opacity. Many AI models, remarkably DNNs, function as "black boxes," making it challenging to interpret the reasoning behind their decisions [84]. The lack of interpretability and transparency raises concerns about trust, accountability, and the possibility of unintended bias. For instance, in healthcare,

understanding the reasoning behind an AI-powered diagnosis is crucial for clinicians to make informed decisions and ensure patient safety [85].Patient safety and clinical trials are major ethical hurdles. For trials to be honest, participants must truly understand the risks before agreeing to join. If these rules are broken, it hurts patients and violates their rights. Even though groups like the FDA have strict rules to protect people, some vulnerable groups still get taken advantage of. To use AI responsibly in healthcare, we need clear rules, experts from different fields working together, and a constant focus on putting the patient first[86].significant ethical and legal challenges, including algorithmic bias, lack of transparency in decision-making, data privacy concerns, and unclear liability frameworks. Regulatory bodies are still adapting to oversee AI applications in pharma, emphasizing the need for standardized guidelines that ensure patient safety without stifling innovation[87].

CONCLUSION

Artificial Intelligence is rapidly transforming the pharmaceutical and healthcare industries by enhancing the efficiency, accuracy, and speed of drug discovery, development, manufacturing, and marketing processes. AI technologies such as Machine Learning, Deep Learning, and Generative AI enable researchers to identify novel drug targets, optimize lead compounds, predict drug safety and efficacy, and streamline clinical trials. In addition, AI supports pharmaceutical product management through market forecasting, pricing strategies, and supply chain optimization. However, the successful implementation of AI requires addressing key challenges, including data availability, model transparency, ethical considerations, and regulatory compliance. AI systems should be viewed as supportive tools rather than replacements for human expertise, ensuring that scientific validation and clinical judgment remain central to pharmaceutical research and patient care. Overall, the integration of Artificial Intelligence into pharmaceutical sciences represents a significant advancement that has the potential to reduce drug development time and cost, improve patient outcomes, and drive innovation in modern healthcare. Continued research, collaboration, and responsible implementation of AI technologies will be essential to fully realize their benefits in the future of drug discovery and pharmaceutical development.

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