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Applications of artificial intelligence and machine learning in pharmaceutical domain: A comprehensive review

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Abstract

Artificial Intelligence (AI) is transforming the medical sector by enhancing diagnosis accuracy, improving treatment outcomes, optimizing healthcare workflows and advancing medical research. Its ability to analyze complex data and assist healthcare professionals has the potential to revolutionize patient care and drive innovation in the field of medicine. Its ability to analyze the amounts of data, identify patterns and make predictions has significantly advanced these fields, leading to improved healthcare outcomes and fostering new avenues for medical research and development. In this review, various applications of AI techniques in healthcare, such as drug design, disease diagnosis, personalized treatment, gene editing and medical education. AI plays a crucial role in disease diagnosis by analyzing medical images, genomic data and patient records, were discussed. AI is transforming medical education by providing personalized and interactive learning experiences. AI algorithms can efficiently analyze large genomic datasets, identifying potential target genes and predicting the outcomes of genetic modifications.

Keywords: Artificial Intelligence; *In silico* studies; AI applications; Drug design; Disease diagnosis; Drug screening

1. Introduction

Artificial Intelligence (AI) is a branch of science that combines intelligent computer programs with machine learning to provide improved outcomes in a variety of scientific and academic domains. Its goals include data analysis, system development and correct analysis. Computational intelligence and statistical models are combined in AI technology. Although redundancy issues are frequently linked to developments in AI applications, their effectiveness benefits the sector. By using AI in a variety of pharmaceutical industry domains, including drug discovery and development, drug repurposing, increasing pharmaceutical production, clinical trials, etc., to mention a few, it is possible to accomplish goals more quickly, while also decreasing the workload of human workers. AI models are useful and affordable in the drug development process because they can predict *in vivo* responses, pharmacokinetics parameters and dosing. The ancient drug discovery process is a long and tedious process that costs a lot of money. The identification of the lead molecules is a lengthy process [1]. New drug discovery processes take a minimum of 20 years. The identification of pharmacokinetic and pharmacodynamic properties of the new molecules is difficult for ancient drug discovery [2]. Target prediction and lead optimization are long processes that are cost-effective. So, 90% of new drug identification is a failure of the drug discovery process [3]. In a normally personalized treatment, the results vary from patient to patient and treatment accuracy was low. Researchers and medical professionals have recently grown increasingly conscious of the fact that every person's illness is unique. Due to the variability of the patient population, some patients may respond better to a certain therapy than others [4]. Scientists must comprehend the pathophysiology of the disease they are trying to treat in order to create a new therapy that works. Despite the fact that many diseases underlying biological

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mechanisms have been discovered over the years, our understanding of diseases as a whole has not kept pace, especially when it comes to disorders of the nervous system. As a result, it is difficult to find effective treatment options for many diseases [5]. The effective treatment of patients is based on the proper diagnosis of the diseases. Disease diagnosis is important for the identification and differentiation of various diseases. The normal diagnosis has low accuracy and is time-consuming [6].

AI is one of the most advanced modern techniques in the medical healthcare system. AI has effectively reduced the lengthy process of drug discovery and its cast. It's identified the lead molecule and target prediction for drug discovery in a low-time-consuming manner. AI improves personalized treatment from patient to patient [7]. AI-based algorithms are useful for locating underdiagnosed or undertreated individuals, unencoded diseases and unusual diseases. Therefore, AI illness diagnostic models offer several opportunities for patient early diagnosis [8]. AI is also used to educate students about healthcare and help them to improve their skills in medical education [9].

If current trends continue, it won't be long before machines rather than people create the medications we consume. AI-enabled drug discovery holds enormous potential to improve access to medications and treat currently incurable illnesses because it promises reduced costs and faster development times. It also creates a whole variety of unresolved problems, such as those involving intellectual property rights, the danger of technical misuse and the ongoing maintenance of drug safety and efficacy in this modern period.

Pre-clinical phases of conventional drug discovery are notoriously lengthy and expensive, spanning three to six years on average and costing hundreds of millions to billions of dollars. However, a variety of AI technologies are revolutionizing almost every step of the drug discovery process, holding great promise for changing the industry's pace and cost. In the target identification stage of drug discovery, artificial intelligence (AI) is being trained on massive datasets, such as omics datasets, phenotypic and expression data, disease associations, patents, publications, clinical trials, research grants and more, to understand the biological mechanisms of diseases and to identify novel proteins and/or genes that can be targeted to treat those diseases. By anticipating the 3D structures of targets and speeding up the creation of effective medications that attach to them, AI can go beyond simple target recognition. By enabling high-fidelity molecular simulations that may be done solely on computers (i.e., *in silico*) without incurring the prohibitive expenses of conventional chemical procedures, AI is also being utilized to lessen the requirement for physical testing of prospective therapeutic molecules. By predicting important qualities like toxicity, bioactivity and the physicochemical properties of compounds, some AI systems are being utilized to avoid simulating the testing of drug candidates.

The paradigm of traditional drug development, which has often entailed screening enormous libraries of potential compounds, is changing as a result of AI. Some systems must be capable of creating potential, previously undiscovered medicinal compounds from scratch. AI is used to rank these molecules and prioritize them for further evaluation when a group of promising "lead" medicinal compounds have been discovered. AI approaches beat earlier ranking techniques. Beyond theoretical medication design, AI is also being used to build synthesis pathways for creating fictitious drug molecules, occasionally suggesting changes to substances to make them more readily producible.

2. AI in drug discovery

The pharmaceutical industry has dramatically increased its data digitization during the last few years. However, the task of gathering, examining and utilizing that knowledge to resolve challenging clinical problems comes along with this digitalization [10]. Because AI can handle massive amounts of data with improved automation, this encourages its use [11]. Artificial intelligence (AI) is a technology-based system that uses a variety of cutting-edge tools and networks to simulate human intelligence. While not totally replacing human physical presence, it does not completely threaten to do so [12,13]. AI makes use of hardware and software that can analyze and learn from input data to make independent decisions for achieving predetermined goals. Acting in accordance with the McKinsey Global Institute, the rapid advances in AI-guided automation will be likely to completely change the work culture of society [14,15].

AI in drug discovery and development demonstrate its potential to accelerate the process, increase efficiency and improve success rates in bringing new drugs to market. However, it's important to emphasize that AI is a tool that complements the expertise of researchers and rigorous experimental validation and regulatory compliance remain essential in the drug development pipeline [16]. The abundance of medicinal molecules is encouraged by the broad chemical space, which contains more than 1060 molecules [17]. However, the drug development process is constrained by a lack of cutting-edge technologies, making it a time-consuming and expensive effort that can be resolved by applying AI [18]. The use of AI can identify hit and lead compounds, validate the drug target more quickly and optimize the design of the drug structure [17,19]. Despite its benefits, AI must contend with serious data difficulties such as the size, expansion, diversity and ambiguity of the data. Millions of molecules may be present in the data sets available to

pharmaceutical corporations for medication development, making them difficult for typical ML systems to handle. Large numbers of chemicals or straightforward physicochemical properties, such log P or log D, can be quickly predicted using a computational model based on the quantitative structure-activity relationship (QSAR). These models, however, are a long way from making accurate predictions about complicated biological characteristics like a compound's effectiveness and unfavorable side effects. Small training sets, incorrect experimental data in training sets and a lack of experimental validations are further issues QSAR-based models encounter. To address these issues, large data modeling and analysis based on recently established AI methodologies can be used to evaluate the safety and efficacy of pharmacological compounds. For absorption, distribution, metabolism, excretion and toxicity (ADMET) data sets of drug candidates, it demonstrated significant predictivity in comparison to conventional ML techniques [20,21].

The vast virtual chemical space hints to a molecular topographic map by showing molecular distributions and characteristics. The concept behind the chemical space visualization is to gather positional data on molecules within the space in order to look for bioactive compounds. As a result, virtual screening (VS) aids in the selection of suitable molecules for further testing. PubChem, ChemBank, DrugBank and ChemDB are a few open-access chemical databases.

Along with structure and ligand based approaches, there are other *in silico* ways to virtual screen compounds from virtual chemical spaces that offer better profile analysis, quicker non-lead compound elimination and faster therapeutic molecule selection at lower cost [17]. The physical, chemical and toxicological properties are taken into account when choosing a lead ingredient via drug design algorithms such coulomb matrices and molecular fingerprint identification [22]. The desired chemical structure of a compound can be predicted using a variety of characteristics, including prediction models, the similarity of molecules, the molecule creation process and the use of *in silico* methodologies [19,23].

The development of AI-based QSAR approaches, such as linear discriminant analysis (LDA), support vector machines (SVMs), random forests (RF) and decision trees, has been used to identify potential drug candidates using QSAR modeling tools [24-26]. These approaches can be used to accelerate QSAR analysis. When King et al. examined the capacity of six AI algorithms to rank anonymous substances in terms of biological activity with that of conventional techniques; they discovered a minimal statistical difference [27].

AI algorithms can analyze large-scale biological and chemical datasets to identify potential drug targets and validate their relevance to specific diseases. By integrating genomic, proteomic, and clinical data, AI can uncover novel therapeutic targets and prioritize them based on their potential for successful intervention [28].

3. AI in drug design

3.1. Prediction of the Target Protein Structure

While designing a drug molecule, it is essential to assign the correct target for successful treatment. Numerous proteins are involved in the progress of the disease and in some cases, they are overexpressed. Therefore, it is crucial to estimate the structure of the target protein while designing the therapeutic molecule in order to selectively target disease. Because the design is in accordance with the chemical environment of the target protein site, AI can help in structure-based drug discovery by predicting the 3D protein structure. This helps to predict the effect of a compound on the target along with safety considerations before their synthesis or production [29]. The basic protein sequence was encoded and the torsional angles for each residue as well as a half-finished backbone derived from the geometric unit upstream of this were then taken into consideration as input and produced a novel backbone as output. The three-dimensional structure was the output of the final unit. The distance-based root mean square deviation (dRMSD) measure was used to evaluate how far the anticipated and experimental structures deviated from each other [30].

Atomic resolution structural information of small molecules binding to drug targets offers opportunities for structure-guided hit identification, fragment screening and ligand optimization. However, structural coverage for only 35% of the human proteome remains underrepresented, especially for pharmaceutically relevant protein target families like G-protein-coupled receptors (GPCRs) and ion channels [31]. Computational structure prediction methods, such as homology modeling, have shown improved success in protein structure prediction even without a template structure [32]. DeepMind, in partnership with EMBL-EBI, has made freely available the 3D structures predicted by AlphaFold2, offering structural coverage for 98.5% of the human proteome. Although these developments signify advancements in protein structure prediction, it is too early to declare AI has cracked the protein-folding problem or its impact on drug discovery will be transformative [33].

3.2. *De novo* drug design

De novo drug design, developed 25 years ago, aims to generate new active molecules without reference compounds. However, it has not gained widespread use in drug discovery due to the difficulty in accessing synthetically difficult compounds [34]. *De novo* drug design as a practice is being superseded by emerging approaches as a result of the former's drawbacks, including challenging bioactivity prediction and convoluted synthesis routes. In addition, computer-aided synthesis planning can forecast a variety of synthesis paths for millions of potential structures. Variational autoencoders, which consist of two neural networks, have been used to train models based on Quantitative estimation of drug-likeness scores and synthetic accessibility scores [35-38]. These models have been compared to adversarial autoencoders, which produce more valid structures.

In order to create products that are chemically practical and have a large rate of reaction, a framework was devised in which a rigorous forward reaction template was applied to a set of reactants. Based on a score provided by the neural networks, machine learning was utilized to identify the dominating product [22]. SMILES strings used to represent molecules were used to train this platform. Then, using specified chemical descriptors for MW, logP and topological polar surface area (TPSA), it produced compounds.

The Reinforcement Learning for Structural Evolution approach, which uses generative and predictive DNNs to create novel molecules, was created for *de novo* drug synthesis. In this case, the predictive models are utilized to forecast the features of the created chemical while the generative model generates more distinctive molecules in terms of SMILE strings based on a stack memory [39]. The involvement of AI in the *de novo* design of molecules can be beneficial to the pharmaceutical sector because of its various advantages, such as providing online learning and simultaneous optimization of the already learned data as well as suggesting possible synthesis routes for compounds leading to swift lead design and development [38,40].

Recursive neural networks (RNNs) have also been successfully used for *de novo* design, using sequential information to generate chemical structures. Reinforcement learning and transfer learning have been applied to bias the generated compounds towards desired properties [41]. Inverse-QSAR modeling, another *de novo* molecular design approach, seeks to design molecules with desired activity or property by inversely mapping the molecular descriptor from a pre-constructed quantitative structure-activity/property relationship (QSAR/QSPR) models [42].

4. AI in drug screening

Drug discovery and development is a money and time-consuming process. Even then, however, nine out of ten medicinal compounds fall short of passing regulatory approval and Phase II clinical trials. Due to their ability to predict *in vivo* activity and toxicity, algorithms including Nearest-Neighbour classifiers (RF), extreme learning machines (SVMs), and deep neural networks (DNNs) are utilized for VS based on synthesis feasibility [43-45]. A platform for the identification of treatments for conditions like immune-oncology and cardiovascular disorders has been developed by a number of biopharmaceutical companies, including Bayer, Roche, and Pfizer, in collaboration with IT firms [17].

When developing a new drug, it is important to take into account how the drug's predicted physicochemical properties, such as solubility, partition coefficient (log P), degree of ionization and intrinsic permeability, may indirectly affect its pharmacokinetics and target receptor family. It is possible to anticipate physicochemical properties using a variety of AI-based methods. For instance, ML employs sizable data sets created during earlier compound optimization to train the program [46]. Molecular descriptors, such as SMILES strings, potential energy measurements, electron density around the molecule and coordinates of atoms in 3D, are used in drug design algorithms to produce workable compounds via DNN and afterward forecast their attributes [47].

The Estimation Program Interface (EPI) Suite, a quantitative structure-property relationship (QSPR) workflow, was created to ascertain the six physicochemical characteristics of environmental chemicals collected from the Environmental Protection Agency (EPA) [46]. The lipophilicity and solubility of several substances have been predicted using neural networks based on the ADMET predictor [48]. The solubility of compounds has been predicted using DL techniques including undirected graph recursive neural networks and graph-based convolutional neural networks [49]. The acid dissociation constant of substances has been predicted in several cases using ANN-based models, graph kernels and kernel ridge-based models [46,50]. Similar to this, cell lines including the Madin-Darby canine kidney cells and the human colon adenocarcinoma (Caco-2) cells have been used to gather data on the cellular permeability of a variety of chemicals, which is then given to AI-assisted predictors [51]. Thus, AI has a significant role in the development of a drug, to forecast not only its desired physicochemical properties, but also the desired bioactivity.

Virtual screening (VS) is a computational technique that offers a complementary and cost-effective approach for hit identification in drug discovery. It prioritizes a subset of compounds for evaluation in a primary assay. AI methods that augment VS approaches have gained attention in drug discovery [52]. Ligand-based virtual screening (LBVS) techniques aim to identify active compounds from a chemical library based on molecular similarity. Predictive modeling for VS is an extension of the classical QSAR modeling paradigm. Access to large volumes of chemogenomics data and advances in ML and DL algorithms have provided new opportunities for QSAR modeling as a VS technique [53]. Over the past decade, there has been a shift to web-based cheminformatics workbenches that streamline and automate ML and DL based QSAR workflows for virtual screening. Structure-based virtual screening (SBDD) is a common computational strategy applied in SBDD, driving many structurally enabled drug discovery programs [54].

5. *In silico* pharmacokinetic and toxicity prediction

In the late 1990s, poor pharmacokinetics of drug candidates led to a paradigm shift within the pharmaceutical industry. *In silico* ADMET modeling aims to assist project teams in designing and selecting novel compounds with superior ADMET properties and directing experimental resources to the most favorable compounds [55]. Pharmaceutical companies have deployed many global *in silico* ADMET models in their discovery pipelines. Early work used linear regression methods, but with the development of machine learning algorithms and large-scale homogenous ADMET data, *in silico* ADMET modeling transitioned to ML based predictive models. Multitask DNNs were more accurate in predicting ADMET endpoints than single-task DNNs and shallow-learning ML methods. However, combining mechanistically unrelated endpoints in a multitask model could lead to poor performance, as the information shared between tasks might not be correlated. Therefore, a prior assumptions of the predictive advantage of multitask DNN over single-task DNNs are a challenge, and both approaches need to be evaluated when developing predictive ADMET models [56].

5.1. Prediction of Bioactivity

The affinity of drug molecules for the target protein or receptor determines how effective they are. The therapeutic effect will not be produced by drug molecules that do not interact with or have no affinity for the targeted protein. In rare cases, it's also feasible that enhanced medication molecules will connect with proteins or receptors they weren't intended to, causing toxicity. As a result, it is essential to forecast drug-target interactions using drug target binding affinity. By taking into account the characteristics or similarities of the drug and its target, AI based approaches can estimate a drug's binding affinity. To determine the feature vectors, feature-based interactions identify the chemical moieties of the medication and the target. By contrast, in similarity-based interaction, the similarity between drug and target is considered, and it is assumed that similar drugs will interact with the same targets. For predicting drug-target interactions, web programs like ChemMapper and the similarity ensemble method are available. It is also possible to take into account drug characteristics from SMILES, ligand maximal common substructure (LMCS), extended connectivity fingerprint or a combination of these [57,58].

A drug's bioactivity also takes into account ADME information. The sites of drug metabolism are determined using AI-based techniques like XenoSite, FAME and SMARTCyp. In addition, software such as CypRules, MetaSite, MetaPred, SMARTCyp and WhichCyp were used to identify specific isoforms of CYP450 that mediate a particular drug metabolism [59].

5.2. Prediction of Toxicity

Any drug's toxicity must be predicted in order to prevent adverse effects. The cost of developing new drugs is increased by the frequent use of cell-based *in vitro* assays as preliminary investigations, followed by animal trials to determine a compound's toxicity. Toxtree, pkCSM, LimTox and admetSAR are just a few of the web-based applications available to assist cut costs. Advanced AI-based methods predict a compound's toxicity based on input features or explore for commonalities between substances. The Tox21 Data Challenge organized by the National Institutes of Health, Environmental Protection Agency (EPA) and US Food and Drug Administration (FDA) was an initiative to evaluate several computational techniques to forecast the toxicity of environmental compounds and drugs [54]. An ML algorithm named DeepTox outperformed all methods by identifying static and dynamic features within the chemical descriptors of the molecules, such as molecular weight (MW) and Van der Waals volume and could efficiently predict the toxicity of a molecule based on predefined 2500 toxicophoric features [60].

eToxPred, which was created using ML, was used to calculate the toxicity and synthesis viability of tiny organic compounds and it demonstrated accuracy of up to 72% [59]. Similar to this, open-source methods used in toxicity prediction include TargeTox and PrOCTOR. The guilt-by-association principle, which states that entities with comparable functional qualities have similarities in biological networks, is used by TargeTox, a biological network

target-based medication toxicity risk prediction method. In order to predict drug toxicity, it can generate protein network data and combine pharmacological and functional features in an ML classifier [61,62]. A 'PrOCTOR score' was created by PrOCTOR, which was trained using an RF model, and which included drug-likeliness characteristics, molecular characteristics, target-based characteristics and characteristics of the protein targets to predict if a medication would fail in clinical trials due to its toxicity. The FDA-approved medications that afterward disclosed adverse drug events were also recognized [63,64].

5.3. Predicting Drug-Target Interactions

The effectiveness of therapy depends heavily on interactions between drugs and proteins. To comprehend a drug's efficacy and effectiveness, anticipating how it will interact with a receptor or protein is crucial. This information also enables medications to be repositioned and avoids polypharmacology. The accurate prediction of ligand-protein interactions made possible by a variety of AI techniques has improved therapeutic efficacy [29,65].

By integrating pharmacological and chemical data and verifying two RF models against well-known platforms like SVM with high sensitivity and specificity, it was possible to predict plausible drug-protein interactions. Additionally, these modes could anticipate relationships between drug and target, which could then be expanded to include associations between target and illness and target and target [66]. This could speed up the drug development process. For determining interactions between a drug and G-protein-coupled receptors (GPCRs), ion channels, enzymes and nuclear receptors (NR) respectively, this is a mixture of four sub-predictors. When this predictor was compared with existing predictors, the former surpassed the latter in terms of both prediction accuracy and consistency [67].

AI's capacity to predict drug-target interactions has also been utilized to help reposition currently available medications and prevent polypharmacology. A medicine that has been repurposed or repositioned is eligible for Phase II clinical trials right away [17]. Re-launching an old drug saves money because it only costs $8.4 million to do so as opposed to $41.3 million to launch a brand-new medicinal entity [68]. The 'Guilt by association' method, which may be applied to networks that are knowledge-based or computationally driven, can be used to predict the novel associations between medicine and disease [69]. Logistic regression platforms, such as PREDICT, SPACE and other ML approaches, consider drug–drug, disease–disease similarity, the similarity between target molecules, chemical structure and gene expression profiles while repurposing a drug [70]. Topotecan, a topoisomerase inhibitor currently in use, has been investigated to anticipate its therapeutic use using cellular network-based deep learning technology. A US provisional patent is now covering this platform. Self-organizing maps (SOMs) are employed in medication repurposing and are within the unsupervised category of machine learning. By training the system on a predetermined number of compounds with known biological activities, they are able to search for novel off-targets for a group of pharmacological molecules using a ligand-based strategy [71]. Drug-protein interactions can also foretell the likelihood of polypharmacology or a drug's propensity to interact with many receptors and cause off-target or adverse effects. In order to create safer medicinal molecules, AI can develop a novel molecule using the principles of polypharmacology [72].

6. AI in chemical synthesis

Compound ideation has a long history, with early structure-based *de novo* design approaches involving automated construction of ligands within receptor binding sites [73]. AI-based generative modeling algorithms have gained popularity in recent years, enabling the generation of synthetically tractable compounds with drug-like properties while satisfying the desired target property profile. Generative chemistry relies on AI-based generative modeling tools to generate synthetically tractable compounds with drug-like properties while satisfying the desired target property profile [74]. Current generative modeling methodologies can be categorized based on the underlying method used for molecular featurization. Recent studies have demonstrated the ability of generative AI to deliver synthetically tractable, novel bioactive molecules that satisfy design objectives [75].

Organic synthesis is a crucial aspect of small molecule drug discovery, as it helps identify molecules with improved properties. Synthesis planning is a key discipline in drug discovery, and various computational approaches have been developed to assist in synthesis planning. Three aspects are predicted: reaction outcome, chemical reaction yield and retrosynthetic planning. Retrosynthetic planning is dominated by knowledge-based systems built on expert-derived rules or automatically extracted rules from reaction databases [76]. Machine learning-based approaches have been described for forward synthesis prediction, which ranks synthetic routes from reaction analysis. Examples include quantum chemical descriptors combined with manual encoded rules and machine learning to predict reactions and their products [77]. Artificial intelligence has also been described for retrosynthetic analysis, using sequence-to-sequence based models for retrosynthetic reaction prediction. The technology is comparable to rule-based expert systems, but large differences have been observed over different reaction classes. A combination of three deep neural

networks and a Monte Carlo tree search for retrosynthetic prediction yielded excellent performance, with medicinal chemists preferring the route proposed by this methodology over rule-based approaches [78].

7. AI in pharmaceutical product development

The subsequent inclusion of a novel therapeutic molecule into an appropriate dosage form with the requisite delivery properties is necessary. The more traditional method of trial and error can be replaced in this area by AI [79]. With the use of QSPR, a variety of computational methods can tackle concerns with stability, dissolution, porosity and other formulation design-related challenges [80]. Decision-support tools operate through a feedback mechanism to monitor the entire process and sporadically adjust it. They employ rule-based systems to choose the type, nature and quantity of the excipients based on the physicochemical parameters of the medicine [81].

The influence of the powder's flow property on the die-filling and process of tablet compression has been studied using a variety of mathematical tools, including computational fluid dynamics (CFD), discrete element modeling (DEM) and the Finite Element Method. The effect of tablet geometry on its dissolution profile can also be investigated using CFD [82,83]. The rapid production of pharmaceutical items may greatly benefit from the integration of these mathematical models and AI.

8. AI in drug repurposing

Artificial intelligence (AI) has been increasingly utilized in drug repurposing efforts, which involve finding new therapeutic applications for existing drugs. AI algorithms can analyze large amounts of data from various sources, including electronic health records, scientific literature and clinical trial databases. By mining this data, AI can identify potential connections between drugs and new therapeutic targets [84]. AI can build predictive models to assess the effectiveness of existing drugs against different diseases or conditions. These models can take into account multiple factors, such as molecular structure, biological pathways and genetic information, to identify drugs with potential repurposing opportunities [85-87].

Through computational simulations and molecular docking techniques, AI algorithms can predict the drug-target interactions, helping to identify promising drug candidates for repurposing [88,89]. AI can analyze databases of known drug side effects to identify unexpected therapeutic effects. By examining patterns and correlations in adverse event data, AI algorithms can uncover potential repurposing opportunities by repurposing drugs based on their shared side effect profiles [90]. AI can analyze biological networks and pathways to identify new connections between diseases and existing drugs. By understanding the complex interactions within biological systems, AI can identify drugs that may affect multiple targets or pathways, making them suitable candidates for repurposing [9]. AI can help optimize clinical trials for repurposed drugs by analyzing patient data, identifying suitable patient populations and predicting treatment outcomes. This can improve the efficiency and success rate of drug repurposing trials. Overall, AI offers a powerful toolset for accelerating drug repurposing efforts by leveraging big data, predictive modeling and advanced computational techniques. These applications have the potential to enhance the discovery of new therapeutic uses for existing drugs, ultimately leading to more effective treatments for a range of diseases and conditions [91,92].

9. AI in clinical trial

Clinical trials take about 6-7 years and entail a substantial financial investment in order to determine the efficacy and safety of a medicinal product in people with a specific illness condition. Only one out of every ten molecules that enter these trials, however, is cleared successfully, which is a significant loss for the industry [93]. These failures may be the result of poor patient selection, inadequate infrastructure and outdated technology needs. With the use of AI, these problems can be minimized because to the abundance of digital medical data that is currently available [94].

The enrolment of patients takes one-third of the clinical trial timeline. The enrollment of qualified patients can ensure the success of a clinical study, which would otherwise result in about 86% of failure cases. By applying patient-specific genome-exposome profile analysis, AI can help in the selection of only a certain diseased population for enrollment in Phase II and III of clinical trials. This analysis can aid in the early prediction of the available therapeutic targets in the patients selected. Preclinical molecular discovery as well as the early prediction of lead molecules, that would pass clinical trials with consideration of the chosen patient population by using other aspects of AI, such as predictive ML and other reasoning techniques, help in the early prediction of lead molecules that would pass clinical trials. The failure of 30% of clinical studies is attributed to patient dropout, which necessitates further recruiting efforts to complete the

experiment, wasting time and resources. By carefully monitoring the patients and assisting them in adhering to the appropriate clinical trial procedure, this can be avoided [17,94,95].

10. AI in diseases diagnosis

AI can aid in the diagnosis of diseases by analyzing medical images, such as X-rays, MRIs and histopathological slides. Deep learning algorithms can detect patterns and anomalies in images, assisting healthcare professionals in identifying diseases at an early stage. AI can also analyze patient data, including symptoms, medical history and genetic information, to support diagnosis and personalized treatment decisions. AI assists clinicians in diagnosing patients with various illnesses, reducing diagnostic time and improving efficiency. By analyzing clinical data from radiology, pathology and biochemical examinations, AI can produce accurate results, transforming traditional medical models. This allows doctors to create more deliberate and reasonable treatment plans based on the patient's condition [96].

10.1. AI in Radiology

Radiology currently plays a role in the diagnosis of practically all diseases as a scientific and intuitive foundation for medical diagnosis. The need for radiological diagnoses is growing rapidly each year, but it takes time to develop medical expertise and the number of doctors with radiation medicine experience is only slowly rising. High occupational pressure and rates of misdiagnosis are seen as a result of the growing imbalance between the supply and demand of medical doctors in this field. AI algorithms can help analyze and interpret medical images such as X-rays, CT scans, MRI scans and ultrasound images. These algorithms can assist in detecting and diagnosing various conditions, including abnormalities, tumors, fractures and other anomalies. AI-based CAD systems can automatically highlight potential abnormalities on medical images, acting as a second pair of eyes for radiologists. These systems can help improve the accuracy and efficiency of radiologists by flagging suspicious areas for further evaluation [97-100].

10.2. AI in pathology

AI algorithms can analyze and interpret pathology images, including histopathology slides, cytology slides and immunohistochemistry slides. These algorithms can assist pathologists in detecting and diagnosing various diseases, such as cancer, infections and autoimmune disorders [101]. AI can help identify abnormal cells, classify tissue types and provide quantitative analysis of biomarkers. AI is particularly valuable in the emerging field of digital pathology, where glass slides are digitized and analyzed using computer algorithms. AI can help automate the scanning and digitization process, making it easier to store, access and share pathology images [102]. This technology enables remote consultations, second opinions and large-scale data analysis for research purposes. AI algorithms can assist in quality control processes in pathology laboratories. They can automatically identify errors or inconsistencies in slides, such as staining artifacts or tissue artifacts, ensuring that high-quality results are produced. This can help improve the accuracy and reliability of pathology diagnoses [103,104].

11. AI in personalized treatment

AI can aid in the development of personalized treatment plans by analyzing large-scale datasets, including genomic data, electronic health records and clinical trial data. Machine learning algorithms can identify patterns and correlations in these data, enabling the prediction of treatment responses and the identification of optimal therapies for individual patients. AI can provide decision support to healthcare providers by offering evidence-based recommendations for treatment options. By analyzing patient data, including medical history, genetic profiles and real-time monitoring data, AI algorithms can assist in identifying the most effective interventions and predicting potential adverse events. This helps healthcare professionals make more informed decisions regarding personalized treatment plans [105].

AI algorithms can continuously monitor patient data, such as vital signs, biomarker levels and disease progression, to assess treatment efficacy in real-time. By analyzing this data, AI can detect early signs of treatment response or failure, allowing healthcare providers to adjust treatment plans accordingly and optimize personalized therapies [106]. AI technologies can enable remote monitoring of patients outside of traditional healthcare settings. Wearable devices and sensors can collect data on patient’s physiological parameters, activity levels and medication adherence. AI algorithms can analyze this data, providing insights into patient health and facilitating remote interventions and personalized treatment adjustments. AI can leverage patient data to develop predictive models that estimate individual risks for diseases or treatment outcomes. By considering factors such as genetics, lifestyle and environmental influences, AI algorithms can identify patients at higher risk for certain conditions and enable proactive interventions or preventative measures [107].

12. Conclusion

The development of AI and its impressive tools continuously aims to lessen the difficulties faced by pharmaceutical companies, having an impact on both the drug development process and the overall lifecycle of the product. This review explains the application of AI in various aspects of health care. These advancements hold great promise for improving healthcare outcomes, enabling precision medicine and accelerating scientific research in the field of medicine. However, it is important to ensure ethical considerations, regulatory frameworks and ongoing research to maximize the benefits and address any potential challenges or risks associated with AI in healthcare. Through thorough market analysis and forecasting, AI can also assist in determining the product's safety and effectiveness in clinical trials, as well as ensure correct positioning and pricing in the market. Despite the fact that there are presently no pharmaceuticals on the market that were created using AI-based approaches and despite the fact that specific implementation issues still exist, it is expected that AI will soon become a crucial tool in the pharmaceutical business.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors declare no conflict of interest.

Authors Contributions

All the authors have contributed equally.

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