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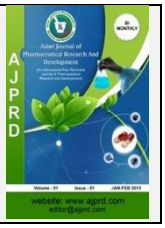

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Review Article

Advances in Artificial Intelligence for Drug Discovery and Development: A Review of Current Trends and Applications

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A B S T R A C T

The rapid advancement of Artificial Intelligence (AI) has revolutionized drug discovery and development, reshaping the pharmaceutical landscape with its computational power and data-driven approaches. AI-driven methodologies, including deep learning, machine learning, and neural networks, have significantly expedited target identification, lead optimization, and drug repurposing, thereby reducing both time and cost associated with traditional drug development. Virtual screening, molecular docking, and predictive modelling have enabled more precise drug-target interactions, enhancing therapeutic efficacy and minimizing potential adverse effects. Moreover, AI's integration into chemical synthesis, polypharmacology, and biomarker discovery has expanded its applications in personalized medicine. This review explores the latest trends and applications of AI in drug discovery, emphasizing its role in optimizing drug design, predicting novel therapeutics, and improving preclinical and clinical trial success rates. While AI has demonstrated remarkable potential, challenges such as data bias, interpretability, and regulatory concerns remain critical barriers to its full-scale implementation. Addressing these challenges will be essential to unlocking AI's transformative capabilities in revolutionizing modern drug development.

Keywords; Artificial Intelligence (AI), Drug Discovery, Machine Learning (ML). Deep Learning (DL)

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INTRODUCTION

The traditional drug discovery process is a complicated and demanding task, often taking up to 15 years and costing between $1 to $2 billion for each drug that gets approved. This is mainly because of increasing failure rates and lengthy clinical trial timelines.[1] Even with substantial resource investments, nearly 90% of drug candidates fail after progressing to phase-I clinical trials. Reaching phase-I clinical trial after extensive preclinical optimization is regarded as a major achievement for both pharmaceutical companies and academic institutions.[2]To improve the success rate of lead compounds in clinical trials, large-scale computational screening and docking techniques have been utilized. However, these methods face challenges like inefficiency and inaccuracy.[3] To address these issues, deep learning (DL) and machine learning (ML) algorithms, which are part of artificial intelligence (AI), have been recognized as promising solutions.[4] These AI tools can predict macrosystem properties with high precision while maintaining low computational costs. As a result, chemical and biological scientists have increasingly embraced AI algorithms in the drug discovery process. AI technologies, such as machine learning (ML) and natural language processing, have the potential to speed up and enhance this process by allowing for more efficient and precise analysis of large data sets.[5] Recent successes in using deep learning (DL) to predict the effectiveness of drug compounds with high accuracy have been reported[6]. These and other research efforts demonstrate AI's potential to enhance the efficiency and effectiveness of drug discovery.Over the past ten years, drug discovery has experienced significant changes, largely fueled by the rapid advancements in artificial intelligence (AI). Common AI applications in drug discovery include virtual screening, de novo drug design, retrosynthesis and

reaction prediction, and de novo protein design.[7-9] To support these AI applications, various AI techniques are utilized, with model architectures transitioning from traditional machine learning models to advanced deep neural networks, including convolutional neural networks, recurrent neural networks, graph neural networks, transformers, and more.

This extensive process, crucial for bringing effective medications into clinical use, includes multiple stages such as target identification, lead compound discovery, optimization, thorough preclinical testing, and careful clinical trials.

Figure 1: The role of AI in pharmaceutical research and drug development

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY:

AI in Drug Designing

In the realm of drug design, artificial intelligence (AI) plays a pivotal role in improving the identification of promising lead compounds, thereby significantly speeding up the drug development process.[10] This progress is facilitated by AI's capacity to evaluate a diverse range of molecular structures and forecast their potential binding interactions, which simplifies the journey from initial concept to clinical application. The core objective of drug design is to uncover small molecules that meet essential criteria, such as therapeutic effectiveness, a safe profile, appropriate chemical and biological characteristics, and the novelty required to obtain intellectual property protection for commercial success[11,12]. Although computational methods have dramatically changed the landscape of drug design, traditional approaches still face issues like lengthy preparation times, substantial computational expenses, and inconsistent dependability. AI emerges as a powerful tool to overcome these obstacles, boosting the efficiency and impact of computational strategies in drug discovery.

A crucial aspect of drug design focuses on studying protein structures, as many diseases stem from protein dysfunction. Structural drug design seeks to identify small molecules that can selectively bind to protein targets. Traditionally, predicting the 3D structures of proteins has been expensive, time-intensive, and often inaccurate [13]. However, AI, particularly deep learning and feature extraction tools, has transformed this field by enabling precise predictions of secondary protein structures and mapping protein contacts. This enhances the understanding of the structure-sequence relationship and aims to improve 3D protein structure predictions, facilitating the study of protein-protein interactions (PPI) and advancing structural drug design. AI's integration into this process marks a significant advancement, promising faster, more cost-effective, and successful drug development.

Figure 2: Benefits of AI in Drug Discovery

Prediction of the Target Protein:

Predicting the three-dimensional (3D) structure of target proteins with precision is a vital step in structure-based drug design and discovery. Machine learning and deep learning, both subsets of artificial intelligence (AI), have become crucial in tackling this challenge. The process of AI-driven protein structure prediction is built on gathering extensive data on protein sequences and structures from various sources. These datasets train AI models to recognize intricate patterns that connect amino acid sequences to their 3D forms [14,15]. By employing advanced computational methods, particularly deep learning, AI models have demonstrated remarkable success in identifying complex patterns within protein data. These models carefully analyze features such as amino acid properties, structural motifs, and evolutionary history to predict 3D protein structures from sequences [16,17]. A significant milestone in this field is AlphaFold, developed by Google DeepMind, which predicts protein structures by examining the distances between amino acids and the angles of peptide bonds. In a notable evaluation, AlphaFold accurately predicted 25 out of 43 protein structures, showcasing its potential to revolutionize structure-based drug discovery. This advancement underscores AI's ability to improve the accuracy, speed, and efficiency of drug design efforts.[18]

Prediction of Drug Protein Interactions:

The prediction of drug-protein interactions (DPIs) is a fundamental aspect of advancing effective drug development, greatly enhanced by the integration of AI. Through the application of advanced computational techniques, such as machine learning and deep learning, AI enables the analysis of extensive biological and chemical datasets [19]. These datasets, carefully organized into comprehensive databases, include detailed information on well-documented DPIs, covering molecular structures, chemical properties, and experimental binding affinities.The study of drug-protein interactions (DPIs) is critically important, particularly as the pharmaceutical industry evolves with the introduction of new therapies and the repurposing of existing drugs for novel clinical uses [20]. Traditional biological methods for developing new drugs are time-consuming and expensive, often taking 10–20 years and requiring significant financial resources. As a result, computational approaches, including AI, have become essential tools for accurately predicting DPIs, speeding up the development of advanced prediction methods. In recent years, the transition from traditional machine learning to more advanced deep learning techniques has transformed DPI prediction. Deep learning models, such as deep neural networks (DNNs), convolutional neural networks (CNNs), and recurrent neural networks (RNNs), have shown superior accuracy compared to earlier methods, driving further research in this area.[21-23].Accurately predicting ligand-protein interactions is vital for understanding therapeutic effectiveness, facilitating drug repurposing, and reducing risks related to polypharmacology. AI has proven highly effective in achieving precise predictions of these interactions, leading to improved treatment outcomes. For example, Wang et al. created a model using the support vector machine (SVM) approach, trained on 15,000 protein-ligand interactions, which successfully identified nine new compounds and their interactions with four key targets based on protein sequences and small molecule structural features.

AI in de Nova Drug Design:

De novo drug design involves the development of completely new drug-like molecules from the ground up, without depending on existing compounds or predefined templates. This method offers significant potential for exploring the expansive chemical space, which is believed to encompass between 10^60 to 10^100 drug-like molecules (Jiménez-Luna et al., 2021). Artificial intelligence (AI), utilizing machine learning and deep learning technologies, has become a crucial tool in overcoming the challenges associated with de novo design, heralding a transformative shift in the discovery of new therapeutic agents [24]. Conventional de novo design approaches often encounter obstacles such as complex synthesis pathways and the challenge of predicting the biological activity of newly created molecules. AI aims to address these limitations by employing advanced computational models and algorithms to analyze vast chemical and biological datasets, identifying patterns that link molecular structures to their pharmacological properties.

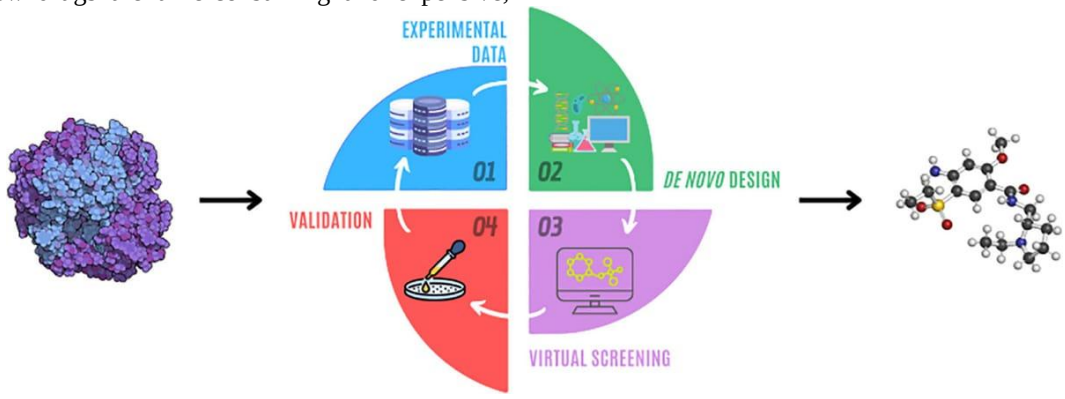

Figure 3: De-Nova Drug design through Artificial Intelligence.

Generative AI models, including variational autoencoders (VAEs) and generative adversarial networks (GANs), have proven highly effective in this field. These models are capable of learning the underlying patterns in molecular representations and producing new chemical compounds with specific, targeted properties[25-27].

The use of AI in de novo drug design goes beyond the creation of small molecules. Advanced methods such as deep neural networks (DNNs) and Monte Carlo tree searches (MTCS), integrated with symbolic AI, have been utilized for predicting chemical reactions and elucidating mechanisms, allowing for faster exploration of chemical space compared

to traditional methods.[28,29] Additionally, AI has demonstrated potential in predicting protein-protein interactions (PPIs), an area with significant therapeutic potential that remains largely unexplored. By analyzing PPI interfaces using AI-driven approaches, researchers can uncover critical structural insights that guide the design of new therapeutic agents targeting these interactions. Despite notable advancements, fully harnessing the capabilities of AI in de novo drug design continues to be an active research focus. Key challenges include accurately predicting the bioactivity of novel molecules, generating compounds that are synthetically feasible, and efficiently navigating the vast chemical space [30,31]. Nevertheless, the incorporation of AI techniques into de novo drug design marks a revolutionary shift, holding promise for accelerating the discovery of innovative, safe, and effective therapeutic agents.

AI in Drug Repurposing:

Drug repurposing, also known as drug repositioning or retasking, refers to the process of discovering new therapeutic uses for drugs originally developed for different medical conditions[32]. This strategy has gained considerable attention due to its ability to speed up the drug development timeline, lower costs, and deliver treatments to patients more quickly than conventional drug discovery methods [33, 34].AI has emerged as a critical tool in drug repurposing, leveraging its advanced analytical capabilities to process vast datasets, including drug databases, clinical records, and genomic information. This enables the identification of new relationships between existing drugs and potential disease targets [35]. AI facilitates drug repurposing through various methods, such as network-based, feature-based, and matrix-based approaches [36]. A major advantage of AI-driven repurposing is the ability to bypass early-phase clinical trials and toxicological evaluations, as the safety profiles of these drugs are already established from prior research. This efficiency allows repurposed drugs to advance directly to Phase II trials for new indications, significantly shortening development timelines and reducing costs [37-38].AI techniques, including deep neural networks (DNNs) and generative adversarial networks (GANs), have demonstrated significant potential in classifying complex drug mechanisms, predicting pharmacological properties, and designing new drug molecules [39-40]. DNNs can categorize drugs based on their functional class, efficacy, therapeutic use, and toxicity, while GANs can create novel molecular structures inspired by real-world data, paving the way for innovative drug design[41,42]. Reinforcement learning, another AI approach, offers a distinct advantage by not relying heavily on pre-existing datasets. Instead, these algorithms can identify strategic patterns in drug molecule design, potentially leading to the development of drugs with fewer side effects. Moreover, AI algorithms can be trained to distinguish between cardiotoxic and non-cardiotoxic drugs, further improving the safety of repurposed medications [43]. Although AI holds immense promise for drug repurposing, several challenges persist, such as the need for extensive computational power to handle and analyse large-scale networks. Furthermore, innovative approaches, like developing machine-learning models centred on drug side effects, could open new avenues for repurposing by identifying specific areas worthy of deeper exploration[44]. The integration of AI into drug repurposing marks a transformative shift in drug discovery, with the potential to accelerate the development of new therapies, reduce costs, and fast-track the availability of effective treatments, particularly for complex and rare diseases that currently lack sufficient treatment options.

AI in Virtual Screening:

Virtual screening is a key computational approach in contemporary drug discovery, facilitating the swift assessment of extensive chemical libraries to pinpoint potential hit compounds for a specific biological target [45-46]. This method generally involves a series of computational steps designed to filter and rank molecules with the desired biological properties from large collections of small molecules[47]. Virtual screening techniques are broadly divided into two categories: structure-based virtual screening (SBVS) and ligand-based virtual screening (LBVS)[45]. SBVS relies on the three-dimensional structure of the target protein to identify molecules that can bind effectively to its active site, often using molecular docking simulations. On the other hand, LBVS uses a set of known active ligands to find similar compounds based on various molecular features, such as two-dimensional fingerprints, pharmacophore models, or three-dimensional shape similarities [45-48]

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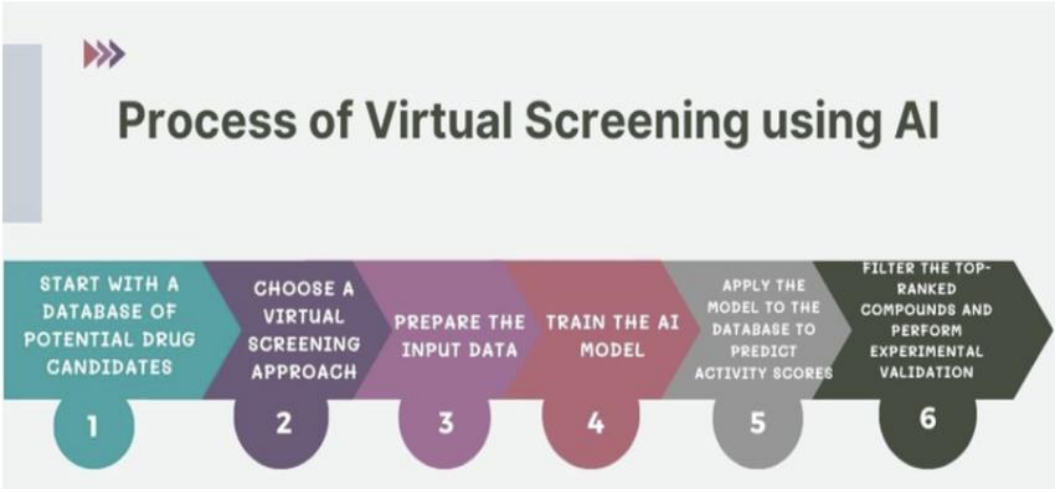

Figure 4: Process of Virtual Screening Using Artificial Intelligence.

Artificial intelligence (AI), especially machine learning and deep learning, has become transformative tool in boosting the efficiency and precision of virtual screening efforts. AI algorithms are capable of analyzing and extracting meaningful insights from the massive datasets produced during virtual screening, such as molecular structures, binding affinities, and target-ligand interactions[45]. In structure-based virtual screening (SBVS), AI techniques like support vector machines (SVMs), random forests (RFs), and boosting algorithms have been used to model complex, non-linear relationships between molecular features and target-ligands interactions, surpassing traditional scoring methods [45]. Deep learning models, including convolutional neural networks (CNNs), have demonstrated exceptional performance in virtual screening by automatically identifying relevant features from molecular data. Tools such as DeepVS and PTPD utilize CNNs for screening compounds against specific targets and designing peptide-based molecules, respectively [49-50]. In ligand-based virtual screening (LBVS), AI methods have proven invaluable for classifying and predicting the bioactivity of compounds based on their physicochemical properties and structural similarities to known active ligands. As the chemical space and available data grow exponentially, deep learning approaches have become essential for efficiently managing large datasets while maintaining speed and accuracy [45].The incorporation of AI into virtual screening provides numerous benefits, such as improved hit rates over conventional screening approaches, the capacity to predict ADME/Tox properties and "drug-likeness" during screening, and the potential to investigate interactions between all known compounds and potential targets. However, it is crucial to emphasize that the results of virtual screening must be validated through appropriate laboratory experiments and clinical studies [51]. AI-enhanced virtual screening has established itself as a vital tool in drug discovery, especially in the search for anticancer agents. Its ability to rapidly screen libraries of natural products—including alkaloids, coumarins, flavonoids, lignans, quinones, tannins, and terpenes—has significantly advanced the identification of promising anticancer lead compounds derived from natural sources [51-52].

AI; Network and Tools

Artificial intelligence (AI) encompasses multiple domains, including reasoning, knowledge representation, and problem-solving, with machine learning (ML) being a key component. ML relies on algorithms that identify patterns within classified datasets. A specialized branch of ML is deep learning (DL), which utilizes artificial neural networks (ANNs). These networks consist of interconnected computational units called "perceptrons," which function similarly to biological neurons by transmitting signals, akin to electrical impulses in the human brain [53]. ANNs are composed of nodes that process inputs and generate outputs, either individually or in complex structures, using algorithms to address various problems [54]. Different types of ANNs include multilayer perceptron (MLP) networks, recurrent neural networks (RNNs), and convolutional neural networks (CNNs), which employ either supervised or unsupervised learning methods[55,56].

The Multilayer Perceptron (MLP) network is utilized in various applications such as pattern recognition, optimization assistance, process identification, and control systems. Typically trained through supervised learning methods that operate in a single direction, MLPs can function as universal pattern classifiers [57]. Recurrent Neural Networks (RNNs), on the other hand, feature closed-loop structures that enable them to retain and store information, exemplified by models like Boltzmann machines and Hopfield networks [57-58].Convolutional Neural Networks (CNNs) consist of dynamic systems with localized connections, defined by their topology, and are widely used in image and video processing, modelling biological systems, simulating complex brain functions, pattern recognition, and advanced signal processing. More advanced architectures include Kohonen networks, Radial Basis Function (RBF) networks, Learning Vector Quantization (LVQ) networks, counter-propagation networks, and ADALINE networks [59]. Figure 1 provides a summary of the diverse method domains within AI.

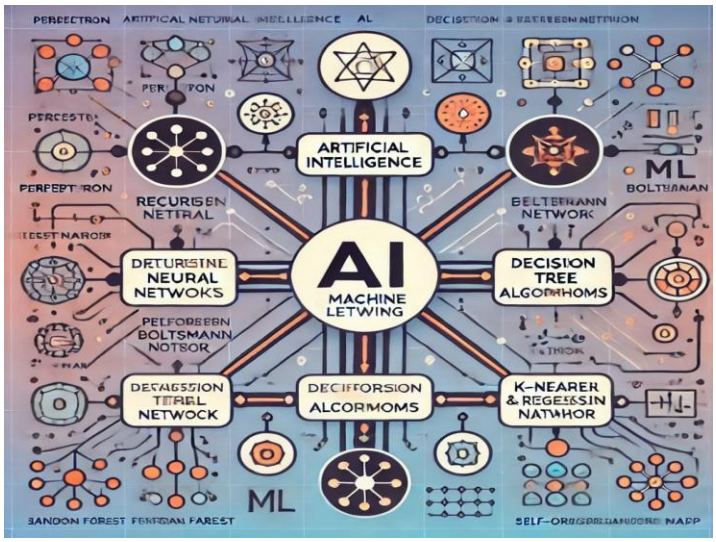

Figure 5: Machine Learning Neural Networks

Numerous tools have been created based on the core architectures of AI networks. A notable example is the International Business Machine (IBM) Watson supercomputer (IBM, New York, USA), which was developed using AI technology. Watson is designed to analyze a patient's medical data and cross-reference it with an extensive database, enabling it to propose tailored treatment strategies for cancer [60-61].

AI in Advancing Pharmaceutical Product Development:

The development of a new drug molecule necessitates its integration into an appropriate dosage form with specific delivery properties. In this context, artificial intelligence (AI) can replace traditional trial-and-error methods [62]. Computational tools, supported by Quantitative Structure-Property Relationship (QSPR) models, can address challenges in formulation design, such as stability, dissolution, porosity, and other issues [63]. Decision-support systems employ rule-based approaches to determine the type, nature, and quantity of excipients based on the drug's physicochemical properties. These systems operate through feedback mechanisms to monitor and adjust the formulation process as needed [64]. Guo et al. combined Expert Systems (ES) and Artificial Neural Networks (ANN) to develop a hybrid system for creating direct-filling hard gelatin capsules of piroxicam, tailored to meet specific dissolution profile requirements. The Model Expert System (MES) provides decisions and recommendations for formulation development based on input parameters, while ANN uses backpropagation learning to correlate formulation parameters with the desired outcomes. These components are managed by a control module to ensure smooth and efficient formulation development [62].Additionally, mathematical tools such as computational fluid dynamics (CFD), discrete element modeling (DEM), and the Finite Element Method have been employed to analyze how powder flow properties affect die-filling and tablet compression processes [65-66]. CFD can also be used to investigate how tablet geometry influences dissolution profiles [67]. Integrating these mathematical models with AI has the potential to significantly accelerate the production of pharmaceutical products.

AI in Pharmaceutical Manufacturing:

As manufacturing processes become increasingly complex, coupled with growing demands for efficiency and superior product quality, modern manufacturing systems are increasingly focused on transferring human expertise to machines, thereby revolutionizing traditional practices [68]. The integration of artificial intelligence (AI) into manufacturing holds significant promise for the pharmaceutical industry. Tools like computational fluid dynamics (CFD), which employ Reynolds-Averaged Navier-Stokes solvers, analyze the effects of agitation and stress levels in equipment such as stirred tanks, enabling the automation of numerous pharmaceutical operations. Similarly, advanced techniques like direct numerical simulations and large eddy simulations address intricate flow challenges in manufacturing [65]. The innovative Chemputer platform facilitates digital automation for the synthesis and production of molecules by utilizing chemical codes and operating through a scripting language called Chemical Assembly [66].

This platform has been successfully used to synthesize compounds such as sildenafil, diphenhydramine hydrochloride, and rufinamide, achieving yields and purity levels comparable to those of manual synthesis [69]. AI technologies also enable efficient estimation of granulation completion in granulators with capacities ranging from 25 to 600 liters [70]. By combining technology and neuro-fuzzy logic, critical variables are correlated with their responses, resulting in a polynomial equation that predicts the required granulation fluid proportion, impeller speed, and diameter for both geometrically similar and dissimilar granulators [71].Discrete element modeling (DEM) has been widely applied in the pharmaceutical industry, for instance, in studying powder segregation in binary mixtures, examining the effects of blade speed and shape variations, predicting tablet trajectories during coating processes, and analyzing the time tablets spend in the spray zone [65]. Artificial neural networks (ANNs) and fuzzy models have been used to investigate the relationship between machine settings and tablet capping, aiming to minimize this issue during manufacturing [72].AI tools such as meta-classifiers and tablet-classifiers help maintain the quality standards of final products by identifying potential errors in tablet manufacturing [73]. Additionally, a patented system has been developed to determine the optimal combination of drug and dosage regimen for individual patients. This system uses a processor to receive patient information and designs customized transdermal patches accordingly [74].

AI in Quality Control and Quality Assurance:

The production of the desired product from raw materials involves balancing several factors [73]. Quality control tests and maintaining consistency between batches often require manual intervention, which may not always be the most efficient approach, highlighting the need for AI integration at this stage [65]. To address this, the FDA updated the Current Good Manufacturing Practices (cGMP) to include a 'Quality by Design' approach, aiming to better understand the critical operations and specific criteria that affect the final quality of pharmaceutical products [75]. Gams et al. combined human efforts with AI by analyzing initial production batch data and creating decision trees. These trees were then converted into rules, which operators used to guide future production cycles [73]. In another study, Goh et al. utilized an Artificial Neural Network (ANN) to analyze the dissolution profile, a key indicator of batch consistency for theophylline pellets. The ANN accurately predicted the dissolution behaviour of the formulation with less than 8% error [76]. AI can also be applied to regulate in-line manufacturing processes to ensure the product meets the desired standards [75]. For instance, ANN-based monitoring of the freeze-drying process, which uses self-adaptive evolution combined with local search and backpropagation algorithms, helps predict temperature and cake thickness at future time points ($t + \Delta t$) under specific operating conditions, ensuring product quality [77]. Additionally, automated data entry platforms like Electronic Lab Notebooks, along with advanced intelligent techniques, can ensure product quality assurance [78]. Data mining and knowledge discovery methods within the Total Quality Management expert system are also valuable tools for making complex decisions and developing new technologies for intelligent quality control [79].

AI in Clinical Trial Design:

Clinical trials aim to determine the safety and effectiveness of a drug for a specific disease in humans, typically spanning 6–7 years and requiring significant financial investment. However, only 10% of drug candidates that enter these trials receive approval, resulting in substantial industry losses [80]. These failures often stem from improper patient selection, inadequate technical resources, and poor infrastructure. Leveraging the vast amounts of digital medical data, AI can help mitigate these issues [81].

Patient enrollment accounts for about one-third of the clinical trial process, and selecting the right participants is crucial, as poor recruitment contributes to nearly 86% of trial failures [82]. AI can enhance patient selection in Phase II and III trials by analyzing genome-exposome profiles to predict suitable drug targets early on. Additionally, AI-driven approaches, including predictive machine learning and reasoning techniques, can assist in identifying promising drug candidates before trials begin, improving the likelihood of success [81].

Figure 6: Artificial Intelligence in Clinical Trial Designing.

Patient dropout rates contribute to 30% of clinical trial failures, necessitating further recruitment efforts and leading to increased time and costs. This issue can be addressed through continuous patient monitoring and adherence support [82]. For instance, AiCure developed mobile application that tracked medication intake in schizophrenia patients during a Phase II trial, improving adherence by 25% and facilitating trial completion

AI in Pharmaceutical Product Management:

AI for product market placement:

Market positioning involves creating a product identity that attracts consumers, making it a key part of business strategies to establish a unique brand [83-84]. This method was used in marketing Viagra, where it was promoted not only for treating erectile dysfunction but also for improving overall quality of life [85].With advancements in technology and e-commerce, companies can now more easily gain brand recognition in the public domain. Search engines are used as a key platform to enhance online visibility and product positioning, as highlighted by the Internet Advertising Bureau. Businesses aim to rank higher than competitors, ensuring quick recognition of their brand [86]. Additionally, techniques like statistical analysis and particle swarm optimization algorithms (introduced by Eberhart and Kennedy in 1995), combined with neural networks, provide insights into markets and help determine marketing strategies based on accurate consumer demand predictions [87].

AI in predicting and analysing market trends:

A company's success depends on its continuous growth and development. Despite having ample funds, pharmaceutical companies are seeing reduced R&D output due to their failure to adopt new marketing technologies [88]. The "Fourth Industrial Revolution" has brought advances in digital technologies, supporting innovative digital marketing through a multicriteria decision-making approach. This method gathers and analyses data, using AI-based models to explore new marketing strategies [89].AI also helps in understanding customer needs and market demands, guiding decision-making with prediction tools. It can forecast sales and analyse the market. AI-driven software engages consumers and informs doctors through ads that link directly to product sites [90]. It also uses natural language processing to analyse keywords and predict purchase probabilities [91-92]. Many B2B companies offer self-service technologies for browsing health products, placing orders, and tracking shipments. Pharmaceutical companies are also launching apps like 1mg, Medline, Netmeds, and Ask Apollo to meet patient needs [89]. Market prediction is crucial for pharmaceutical distributors, who use AI tools like "Business Intelligent Smart Sales Prediction Analysis" to forecast sales and manage stock, preventing overstocking or shortages [93].

AI in optimizing product prizing:

The final price of a pharmaceutical product is determined based on market analysis and the costs incurred during its development. The key idea behind using AI to set this price is its ability to replicate human expert judgment in evaluating the factors influencing product pricing after manufacturing [94]. These factors include research and development costs, regulatory price controls in the relevant country, the length of the exclusivity period, the market share of the new drug before patent expiration, the price of reference products, and price-fixing policies, all of which influence the cost of branded and generic drugs [95].

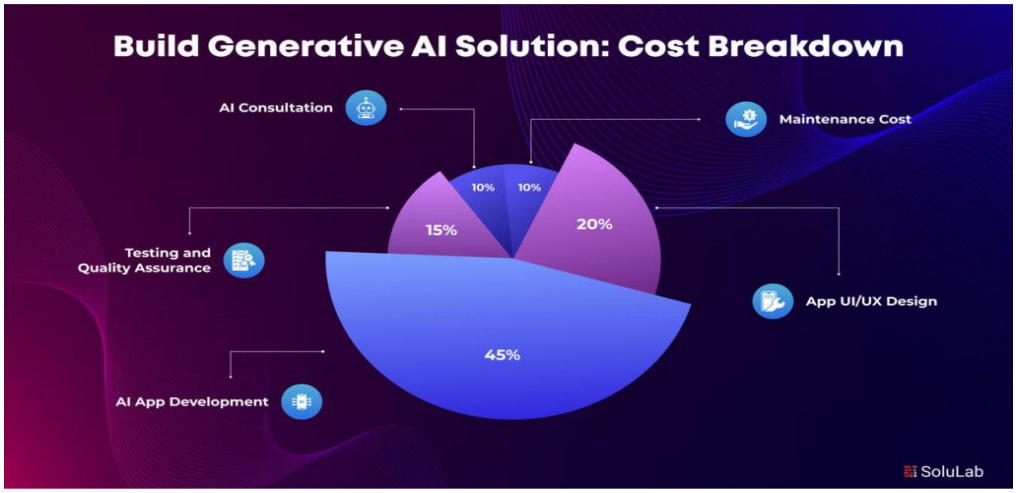

Figure 7: AI in product price optimization.

In machine learning (ML), software analyses large datasets that include product development expenses, market demand, inventory costs, manufacturing costs, and competitor prices, then develops algorithms to predict the product's price. AI platforms like In Competitor, launched by Intelligence Node in 2012, provide a comprehensive retail competitive intelligence service that analyses competitor pricing data, helping brands and retailers monitor the competition. Similarly, platforms like Wise Athena and Navetti Price Point assist users in determining optimal product pricing, suggesting that pharmaceutical companies can adopt these tools to support product costing [96].

Applications of AI in Drug Discovery & Development:

AI in Nanomedicine:

Nanomedicine leverages nanotechnology and pharmaceutical science to diagnose, treat, and monitor complex diseases such as HIV, cancer, malaria, asthma, and inflammatory conditions. In recent years, nanoparticle-based drug delivery systems have gained significant attention in therapeutics and diagnostics due to their ability to enhance treatment efficacy and precision [97]. The integration of artificial intelligence (AI) with nanotechnology holds immense potential to address challenges in formulation development, offering innovative solutions to improve drug delivery and therapeutic outcomes[98].

Nanorobots in Drug Delivery:

Nano robots are composed of integrated circuits, sensors, power supplies, and secure data storage systems, all managed through advanced computational technologies like artificial intelligence (AI) [99-100]. These nanorobots are programmed to perform critical functions such as collision avoidance, target identification, detection and attachment, and eventual excretion from the body. Recent advancements in nano- and microrobotics have enabled these devices to navigate to specific target sites based on physiological conditions, such as pH levels, thereby enhancing treatment efficacy while minimizing systemic side effects [100]. The development of implantable nanorobots for controlled drug and gene delivery requires careful consideration of parameters like dose adjustment, sustained release, and controlled release mechanisms. AI tools, including neural networks (NNs), fuzzy logic, and integrators, play a crucial role in automating these processes [101]. Additionally, microchip implants are utilized for programmed drug release and to track the location of the implant within the body, further enhancing precision and control in therapeutic applications.

AI in Combinational Drug Delivery:

Numerous drug combinations have been approved and commercialized for treating complex diseases like tuberculosis (TB) and cancer, as they can produce synergistic effects that accelerate recovery [102-103]. However, identifying the most effective and precise drug combinations involves high-throughput screening of a vast number of candidates, making the process highly labor-intensive. For instance, cancer therapy often requires a combination of six or seven drugs. Advanced computational tools, such as artificial neural networks (ANNs), logistic regression, and network-based modeling, can streamline the screening of drug combinations and optimize dosing regimens [102-104]. For example, Rashid et al. developed a quadratic phenotype optimization platform to identify optimal combination therapies for bortezomib-resistant multiple myeloma. This platform evaluated a library of 114 FDA-approved drugs and identified decitabine (Dec) and mitomycin C (MitoC) as the most effective two-drug combination. Additionally, the combination of Dec, MitoC, and mechlorethamine was found to be the superior three-drug therapy [103]. Such approaches demonstrate the potential of computational models in enhancing precision medicine for complex diseases.

Figure 8: Applications of AI in Drug Development.

AI for Personalized Drug Dosing:

Historically, clinical practice has followed a "one-size-fits-all" approach to therapy. However, drugs can metabolize differently in different patients, meaning a treatment effective for one group may be less effective or cause adverse reactions in another. These variations are largely due to differences in individuals' genetic profiles. As a result, a more forward-thinking approach has emerged: personalized treatment, also known as precision medicine. This strategy tailors therapies and dosages to an individual's genetic makeup, aiming to optimize treatment outcomes while reducing side effects. Treatments are customized for individuals or groups with similar genetic characteristics. Artificial intelligence (AI) has played a pivotal role in advancing the development of personalized medicine [105].

AI In Drug Toxicity Prediction:

Artificial intelligence (AI) has become a crucial tool in enhancing drug toxicity prediction, significantly improving the ability to identify potential adverse effects of new drug candidates. Through rigorous training and validation, AI models effectively outline toxicity profiles, particularly focusing on potential harm to specific organs or biological pathways. This ability allows for the prioritization of compounds with fewer adverse effects, thereby refining the selection of safer drug candidate[106-107]. Furthermore, the use of AI for toxicity prediction has introduced efficiencies in evaluating off-target toxicity, genotoxicity, organ toxicity, cytotoxicity, and mitochondrial toxicity. By utilizing extensive datasets, including gene expression and cell imaging data, AI models can predict in vivo toxicity effects with high precision. Quantitative Structure-Activity Relationship (QSAR) models, which use ensemble techniques like Random Forests (RF) and Support Vector Machines (SVMs), have demonstrated remarkable accuracy and robustness in toxicity prediction, outperforming traditional methods [108-110].

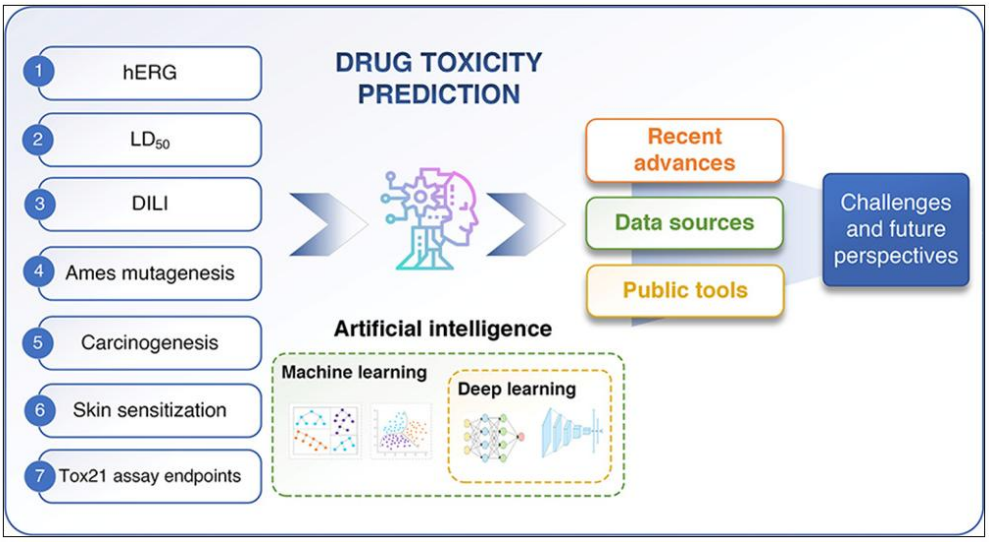

Figure 9: AI in Drug toxicity prediction.

Challenges in Adopting AI: ways to overcome

Despite the immense potential of AI to revolutionize drug discovery, several significant challenges must be overcome to fully realize its capabilities. A major obstacle is ensuring data quality and accessibility. AI models rely heavily on data, and their performance depends on the volume and diversity of the datasets they are trained on. However, obtaining high-quality biological data is often challenging due to privacy regulations and the fragmented distribution of data across various institutions. Moreover, generating the required data can be costly and time-intensive, particularly for smaller research teams. As a result, fostering collaboration and establishing data-sharing initiatives are critical to providing access to comprehensive and diverse datasets, which are essential for advancing AI-driven drug discovery [111-112].Data bias and limited generalizability present significant challenges in AI-driven drug discovery. When trained on biased datasets, AI models can produce unreliable predictions. Such biases might stem from underrepresentation of specific populations in clinical trials, regional variations in data collection, or inconsistencies in healthcare record-keeping practices. Furthermore, overfitting—where a model performs well on training data but poorly on unseen data—can lead to the selection of ineffective drug candidates or false positives. Addressing these challenges is crucial to enhance the reliability and widespread applicability of AI in drug development [113-114].Over time, certain tasks in drug development, manufacturing, supply chains, clinical trials, and sales will become automated. However, these applications fall under the umbrella of 'narrow AI,' which requires extensive training on large datasets and is designed for specific tasks. As a result, human involvement remains essential for the effective implementation, development, and management of AI systems. Concerns about job losses may be overstated, as AI is primarily replacing repetitive tasks, allowing humans to focus on more complex problem-solving, creativity, and strategic insights.

Pharmaceutical companies must gain a clear understanding of AI technology's potential in addressing challenges post-implementation, as well as define realistic and achievable objectives. To fully harness the capabilities of AI platforms, it is crucial to develop a team of skilled data scientists and software engineers who possess strong expertise in AI technology. Additionally, these professionals must have a deep understanding of the company's business targets and R&D goals to ensure the technology is effectively aligned with organizational priorities.

CONCLUSION:

The integration of Artificial Intelligence (AI) into drug discovery and development has become a pivotal milestone in the pharmaceutical industry, significantly enhancing the quality and effectiveness of therapeutic solutions. AI has not only accelerated the drug discovery process but also created new opportunities for drug repurposing, target identification, and predicting novel therapeutic applications. Its crucial role in repurposing has redefined traditional approaches to drug discovery, establishing AI as an essential tool for innovative treatment development. The use of AI in virtual screening and drug design highlights its ability to optimize drug development strategies. By harnessing AI's computational power, researchers can accurately identify and classify target cells, facilitating precise evaluation of potential drug candidates. This efficiency also extends to areas such as polypharmacology, chemical synthesis, and drug repurposing, underscoring AI's transformative impact on advancing global healthcare outcomes.

Conflict of Interests

The authors declare that they have no conflict of interest.

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