STM JOURNALS

International Journal of
Bioinformatics and Computational Biology

ISSN: 2583-9977
Volume 2, Issue 2, 2024
July—December
DOI (Journal): 10.37591/IJBCB

https://journals.stmjournals.com/ijbcb

Review IJBCB

Use of AI Tools to Create New Drugs

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Abstract

The emergence of artificial intelligence in pharmaceutical research [in drug discovery] is a revolution in pharmaceutical research, often combining computational methods with traditional research methods to solve problems. This review article describes various applications of artificial intelligence at various stages of drug development and highlights significant advances and approaches. He explores the critical role of intelligence in drug design, polypharmacology, drug synthesis, drug repurposing, and prediction of drug properties, such as toxicity, biological activity, and physicochemical properties. Although the progress in artificial intelligence is encouraging, this article also addresses the challenges and limitations facing the field, including data quality, performance, computational capability of theory, and ethical reasoning. Providing a broad overview of the role of artificial intelligence in drug discovery, this article highlights the potential of this technology to improve drug development while also acknowledging the challenges that must be overcome to achieve its results.

Keywords: Three-dimensional (3D), Drug–protein interactions (DPIs), artificial intelligence (AI), variational autoencoders (VAEs)

INTRODUCTION

Drug discovery involves the complex process of designing, analyzing, and developing new drugs designed to improve human health and prevent disease. This journey involves several stages, from target identification and discovery to refinement, preclinical testing, and quality control trials, to bring good medicine to clinical practice (Figure 1) [1–4]. Traditionally, this process has required a great deal of time and effort. Despite these efforts, these methods are quite useful and significant benefits to modern medicine, and persistent problems in the treatment of chronic diseases, such as diabetes and cancer [5–8].

Details are in the caption following the image in Figure 1.

The emergence of artificial intelligence (AI) heralds a revolution in medicine that will deliver advanced computing techniques designed to replace human capabilities [9–12]. That is, revolutionary. This technology has the potential to make the drug discovery process more efficient, from computational chemistry and molecular biology to optimization and clinical trial control, molecular dynamics (MDs) simulations, virtual analyses, and new drug design with unprecedented accuracy, opening new therapeutic opportunities and accelerating the identification of promising drug candidates [13–17].

Additionally, the role of AI in systems pharmacology, drug–drug interaction prediction, and

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Received Date: November 14, 2024
Accepted Date: November 27, 2024
Published Date: December 28, 2024

Citation: R. Ganesh. Use AI Tools to Create New Drugs. International Journal of Bioinformatics and Computational Biology. 2024; 2(2): 22–49p.

clinical trials is advancing drug development strategies. Technology is helping to improve patient selection, monitor patient response at the point of care, and streamline processes to improve trial performance and outcomes. However, it is important to combine the wisdom of intelligence with the right balance to ensure that the decision is fair, legal, and rigorous research. Messy. It shows how AI can enable the development of new treatments, streamline clinical trials, and ensure good safety in drug manufacturing. This article advocates the use of AI in drug research and highlights the potential of AI to provide lifesaving and effective global health.

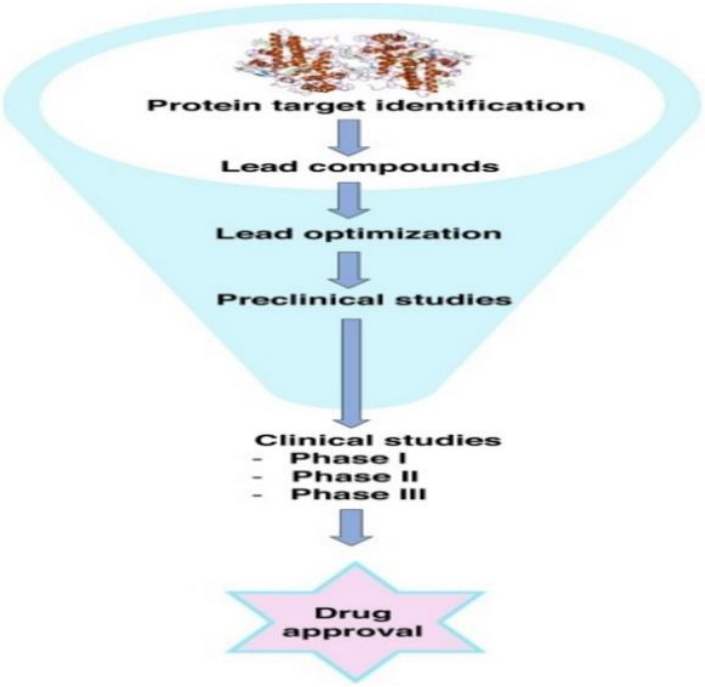

Figure 1. A flow chart of typical drug discovery.

Application of AI in Drug Discovery

AI is revolutionizing drug discovery, increasing efficiency, reducing costs, and improving productivity. The use of AI in all stages of the drug development process (Figure 2).

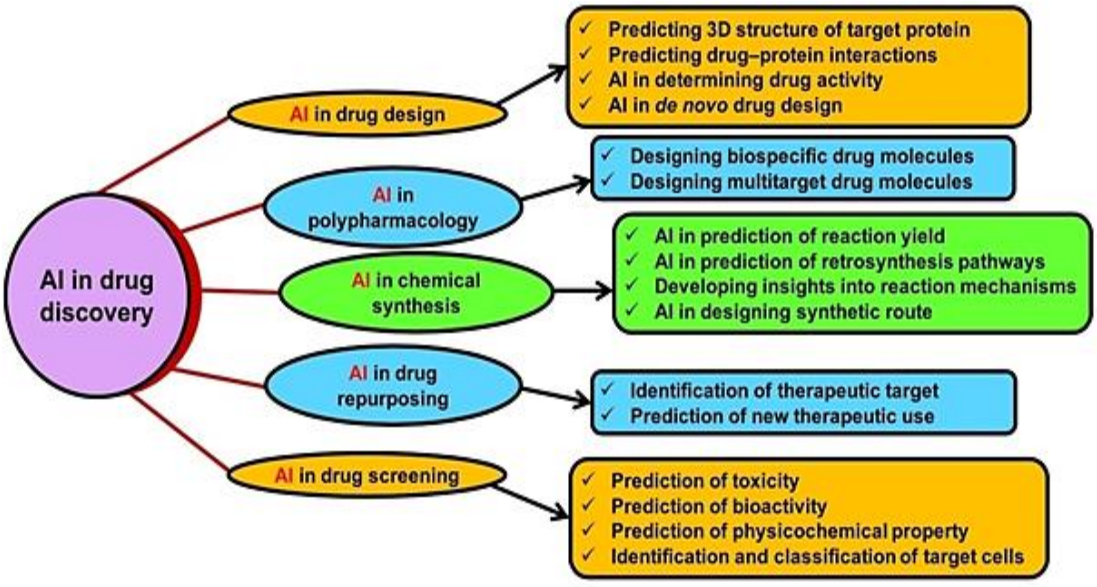

Figure 2. The role of AI in drug discovery.

The integration of AI technology has revolutionized pharmaceutical research by using the best AI in data processing, pattern recognition, and decision making. How can AI technology be used to improve and innovate key areas of drug development, including drug design, polypharmacology, drug synthesis, drug repurpose, and drug screening [18–21]?

Drug Design

In pharmaceutical manufacturing, AI has improved the process of identifying effective products and accelerated the life of drugs[1]. These include the effectiveness of the drug, its safety quality, the required chemical and biological properties, and the innovation required to ensure that the property is a complete job [1, 16]. The approach has faced many problems [22–24], AI stands out as a solution that can overcome these problems and increase energy use and technology efficiency in pharmaceutical manufacturing.

An important application in medicine is the study of the structure of proteins since many diseases are related to the function of proteins. Chemical modeling aims to identify small molecules that selectively interact with protein targets. Traditionally, predicting the three-dimensional (3D) structures of proteins has been expensive and time-consuming, and the accuracy of 3D structures prediction from the outset is limited.

Design Directions

These techniques lead to accurate predictions of protein secondary structures and protein contact maps, improving our understanding of the relationship between structure and sequence. Interactions (PPI) and increasing levels of drug production [26–28].

Prediction of the 3D Structure of the Target Protein

Accurately predicting the 3D structure of a target protein is a key step in drug design and discovery. Machine learning and deep learning algorithms based on intelligence methods have become important tools in solving this challenge. This data allows AI models to be trained to recognize complex patterns that connect amino acid sequences and their 3D structures.

AI models using advanced computational techniques, especially those based on deep learning, have shown great potential in identifying complex patterns in protein data. Historically significant features and using these features to predict protein 3D structures visualized from protein spectra. Distance and proximity of peptide bonds to predict protein structure. Success demonstrates its potential in drug discovery models [29–33].

When correct, routine methods of determining the structure of the protein can often be used. This advancement allows for the creation of drugs based on the structure of the target protein, facilitating early prediction of drug efficacy and safety [34]. Repositories, such as the Protein Data Bank (PDB) and the Drug Bank are used to study the stability, dynamics, geometry, and functional interactions of protein-drug complexes, providing a better understanding of how interactions affect time. Relational modeling also holds promise for analyzing biomedical data using graphical machine-learning techniques. Complex models and drug-effect relationships can help improve drug reproducibility and predict response [35–38].

Prediction of Drug–Protein Interactions

Prediction of drug–protein interactions (DPIs) is the foundation for driving efficient and effective drug development through the integration of AI [39, 40] and chemical data. Such repositories provide a rich learning environment for AI algorithms to identify and learn the complex patterns and relationships that govern interactions between drug compounds and protein targets [41].

AI models are good at identifying key elements that affect DPI by analyzing molecular data, allowing them to predict interactions among new drug users based on their chemical composition. This speeds up the drug development process [39–44].

Research on DPIs plays an important role, especially as the pharmaceutical industry continues to evolve with the introduction of new treatments and the repurposing of existing drugs for new therapeutic uses. The work is long and expensive, often taking 10–20 years and requiring significant financial investment. Development of the pathway [45, 46].

In recent years, the transition from traditional machine learning techniques to more sophisticated deep learning approaches has revolutionized DPI estimation. Deep learning methods, such as deep neural networks (DNNs), convolutional neural networks (CNN), and recurrent neural networks (RNNs) have proven to be more accurate than traditional methods and have achieved further progress in DPI estimation. [45, 47–50]

Accurate prediction of ligand–protein interactions is essential for understanding therapeutic efficacy, ensuring drug reproducibility, and reducing the risks associated with polypharmacology. It is invaluable in ensuring treatment success. For example, Wang et al. developed a model using the support vector machine (SVM) approach and studied 15,000 proteins–ligand interactions; this model identified 9 novel compounds and their interactions with 4 channels as protein structure and structure of the small structure [10, 51, 52].

Furthermore, the technology can help create new molecules based on polypharmacological principles and support the creation of safer drugs, considering that the benefits are not good for linking multiple compounds to multiple targets and off-targets. Furthermore, Bayesian classifiers and SEA algorithms can be used to establish a connection between the pharmacological properties of a drug and its possible targets, enhancing the understanding and prediction of DPIs [10, 53].

AI in de Novo Drug Design

De novo drug design allows the creation of new drug-like molecules from scratch, without relying on pre-existing compounds or structures. Drug molecules. AI, through machine learning and deep learning, plays a key role in overcoming the challenge of new design and aims to revolutionize the discovery of new drugs. Synthetic methods and problems in predicting the activity of new biological molecules. AI tries to overcome these limitations by using state-of-the-art business models and techniques to investigate chemical and biological data to find patterns that connect molecular patterns in terms of their pharmacological properties [10, 54–58].

Generative AI models, such as variational autoencoders (VAEs) and generative adversarial networks (GANs) have shown great success in this field. This model can study the distribution of molecular representation and generate new drugs with desired properties. The VAE-based method aims to continuously incorporate the chemical structure into the latent space to generate new molecules by optimizing the latent representation. Reinforcement Learning System for Evolution (RLSE) uses the DLNS generation and prediction method to develop new molecules and uses newly proposed models and predictive models to evaluate them. The DRL approach has been proven successful in developing molecules with specific targets, such as retinol X and PPAR agonists that meet therapeutic needs. To improve the computer-aided synthesis planning method, introduce syntheses to improve the performance of lead compound discovery and optimization. This is done through the online learning process, continuous improvement of knowledge, and the planning process [10, 20, 24, 59–64].

The use of AI in new drug design extends beyond small molecule production. Techniques, such as DNNs and Monte Carlo tree search (MTCS) have been used in combination with AI for reaction prediction and annotation, allowing for faster chemical identification than traditional methods [65, 66]. Additionally, AI holds promises for predicting PPIs, an understudied area of clinical intervention. By examining PPI interactions with an intelligence-driven approach, researchers can better understand the decision-making processes that govern these interactions and thus inform innovations in PPIs. Although significant progress has been made, realizing the full potential of AI in new drug

development remains an area of research. Challenges include predicting the biological activity of new molecules, designing synthetic compounds, and exploring large chemical spaces. This approach provides the ability to accelerate the discovery of new, safe, and effective treatments [24, 63, 65–68].

AI in Polypharmacology

The drug discovery landscape has undergone a major shift from a one drug, one target a culture to the practice of polypharmacology, a concept that explores interactions between drugs with multiple targets. Treatment is effective and can solve complex disease problems. The adoption of biologics relies on a better understanding of disease mechanisms and the molecular complexities involved. These resources contain a wealth of information about molecular pathways, interactions, and chemical properties, providing a rich tapestry for AI algorithms to explore and make decisions in a variety of ways [19, 53, 69, 71, 72].

The impact of intelligence is being seen with the development of platforms, such as Deep DDI, which aims to show interactions between drugs and predict the use of alternative treatments while reducing adverse events. In addition, AIâ€ ™s predictive capabilities continue to identify target interactions, improve our understanding of drug interactions, and lead to safer, better treatments. This leads to the prediction, forecasting, and engineering of multidrug resistance (MTD) to target attack. Computational techniques driven by AI show great promise in predicting polypharmacological profiles and facilitating drug repurposing (the process of finding new uses for existing approved drugs) [19, 71, 72].

The shift to polypharmacology was driven by the recognition that targeting multiple components of a disease in combination, particularly in multifactorial diseases, may be more effective than targeting a single component. This method includes methods, such as conjugation, replication, and pleiotropy of biological connections and provides greater insight into drug discovery. Time and cost can be reduced by using existing drug approvals in drug development for new drugs. Successful examples of drug transitions have been reported in the literature, and cognitive processes can help identify new opportunities [19].

AI in Chemical Synthesis

The efficiency and stability of drug synthesis are important in drug discovery. The combination of intelligence and chemistry is expanding the scope of drug discovery by leading to the rapid synthesis of drug molecules [73].

The incorporation of AI into drug synthesis addresses an important principle of drug development, improving the efficiency and precision of the synthesis process.

Aspect Synthesis

This is achieved through the combination of automation, real-time reaction analysis, and intelligence, which provides a significant improvement in the speed and reliability of test runs. Challenges, particularly the risk of oversimplifying the inherent complexity of the reaction. This simplification can lead to misunderstanding and interpretation of reaction kinetics and highlights the need to carefully combine AI tools with a deeper understanding of drug content [73, 74–76].

AI in Retrosynthesis Route Prediction

The integration of AI into the field of chemical synthesis, especially retrosynthesis, is a significant step in drug discovery. Using advanced learning technology and deep learning, specialized intelligence can be extracted from vast amounts of data on vaccines. This capability helps to expand the retrosynthetic pathway, which is important in the construction of new drugs.

Complex Structures and Connections

As a result, these models can describe overreaction processes, functional group changes, and bond cleavages, all of which are important in predicting the possibility of returning electronic products to

special purposes. Systematic retrosynthetic approach. It opens the way for synthetic programs. In addition, AI can facilitate the discovery of new synthetic methods by revealing other retrosynthetic strategies that human chemists cannot discover [24, 71, 77–79].

Significant progress in AI has led to the development of machines that can perform better with high accuracy. For example, 3.5 million reactions were used to train DNN, resulting in superior accuracy in predicting reactions and backtesting. Knowledge-based technology. Additionally, neural array-to-array modeling supports accuracy even when examining specific data, such as those in US patents. Antibodies are repurposed for starting products, toward simpler precursors. This work involves single-step and multi-step retrosynthetic prediction to identify potential products by combining them to form target molecules from simple components [60, 77, 78, 80, 81].

Advances in retrosynthetic analysis have evolved from heuristics based on human intelligence to methods based on AI, providing new ways to implement planning that are simple and easy to implement. Traditional methods are limited by their reliance on previous vaccine models and often have general problems with new molecular models and vaccine types. Overcoming these limitations and providing global predictions at a greatly reduced cost, and general sciences (e.g., chemistry, information science) and natural products. The transition to intelligence-driven retrosynthesis is an important step toward more logical, systematic, and effective drug combinations, highlighting the critical role of technology in the future development of drug research [77–78, 82, 83].

AI in Drug Repurposing

Drug repurposing, also called drug repurposing or repurposing, involves identifying new therapeutic applications for drugs developed for other conditions. Get drugs to patients faster than the drug discovery process (Figure 3). Table 1 also shows the key benefits and complications of repeated drug use [84].

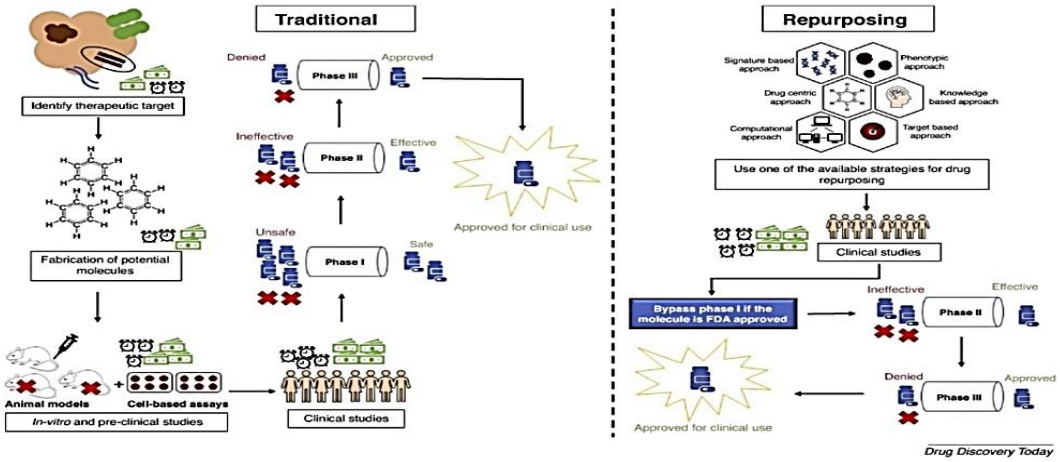

Figure 3. A comparison of traditional drug discovery process versus drug repurposing [84].

AI has become a major force in regenerative medicine by using its deep capabilities to analyze a wide range of data including drug libraries, medical records, diseases, and genomic understanding. These analyses suggest new combinations of existing drugs and new disease targets. The main benefit is that it eliminates the need for early clinical trials and toxicology tests, given that previous studies have established the safety of these drugs. This efficiency allows repurposed drugs to go directly to phase II trials for new indications, reducing development time and money [71, 85–90].

AI technologies, such as DNN and GANs show great potential in classifying complex drug applications, predicting drug properties, and designing new drug molecules. Drugs are divided into therapeutic groups [71, 91, 92].

Table 1. Significance and challenges of drug repurposing.

S.N.	Significance	Reference	Challenges	Reference
1.	Ensures safety.	[96]	Lack of knowledge of regulatory requirements.	[97]
2.	Saves time and money.	[98]	Lack of financial motivations.	[97]
3.	Marketing potential: A higher global revenue stream stimulates market growth.	[96]	Problems in clinical trials: Chance of failure of proof of studies for a new indication.	[98, 99]
4.	Out licensing probability: toward a new indication retaining the rights for the original Indication.	[96, 100]	Intellectual property-related issues hinder the commercialization of repositioned molecule.	[98]
5.	Address unmet medical needs: identifying the new uses for old drugs to treat rare diseases and to target cancers with non-cancer drugs.	[97, 101]	Demands market analysis.	[102, 103]

RL is another AI technique that has the unique advantage of reducing the dependency on knowledge sets for learning. Instead, these algorithms identify good patterns in the design of drug molecules, enabling the creation of drugs with fewer side effects. Additionally, smart algorithms can be trained to distinguish between cardiotoxic and non-cardiotoxic drugs, thus improving the safety of repurposed drugs [71, 93].

Additionally, AI has demonstrated its potential in precision medicine by creating drug molecules that target genetic traits and disease subtypes. This personalized approach is expected to improve treatment outcomes and reduce adverse events.

In the era of big data and online medicine, intelligence technology provides the technology to search for information, identify diseases, medicine, treatment, and determine the target with less error. For example, published reports and information on the relationship between biological pathways and targets have been used to identify drug users for diseases, such as COVID-19 [74, 94–100].

Although AI has great potential for drug recycling, challenges remain, including the need for large financial resources to manage and analyze large networks. Additionally, new strategies, such as developing training models that focus on side effects, could identify specific areas where further research is needed and find new ways to repurpose drugs.

AI in Virtual Screening

Virtual analysis is a computational concept that plays an important role in modern drug discovery. It allows rapid screening of large chemical libraries to identify potential compounds against specific biological targets. The SBVS technique uses a 3D model of the target protein to identify molecules that can effectively bind to its active site, usually using molecular docking simulations, a 2D fingerprint, pharmacophore structure, or similar 3D [104–108].

AI, especially in machine learning and deep learning, has become a powerful tool to improve the efficiency and accuracy of virtual inspections. AI algorithms can process the large amount of data generated during virtual screening and obtain useful information including molecular structure, binding affinity, and target–ligand interactions. AI method and augmentation algorithms were used to establish the relationship between molecular structure and target–ligand interaction, thereby improving the traditional score [104, 109, 110]. Words demonstrate their effectiveness in screening the artifact. Tools like DeepVS and PTPD use CNNs to generate peptide-based molecules to analyze and predict specific content, respectively. As the chemical field and materials continue to expand, deep learning has become essential to process large amounts of data without sacrificing speed and accuracy [104].

The integration of AI in virtual screening has many advantages over traditional screening, such as higher ratings, the ability to predict ADME/Tox products and drug relationships during screening, and the ability to discover interactions of all compounds present. All possible targets. However, it is worth noting that virtual screening results must be supported by appropriate experiments and clinical studies to be more useful. Anti-cancer drugs. The ability to rapidly analyze products, such as alkaloids, coumarins, flavonoids, lignans, quinones, tannins, and terpenes can aid in the identification of antimicrobial agents in natural environments [111, 112].

AI in Pharmaceutical Analysis

Pharmaceutical analysis involves the identification, determination, quantification, and purification of drugs, and plays an important role in the drug discovery process. It relies solely on various testing methods and methods. Although these methods are accurate, the costs of screening new drug candidates from natural products are still high. In contrast, the computational method provides better results. Therefore, AI technology is increasingly used in conjunction with traditional testing [7, 114] to improve drug analysis, shown in Figure 4.

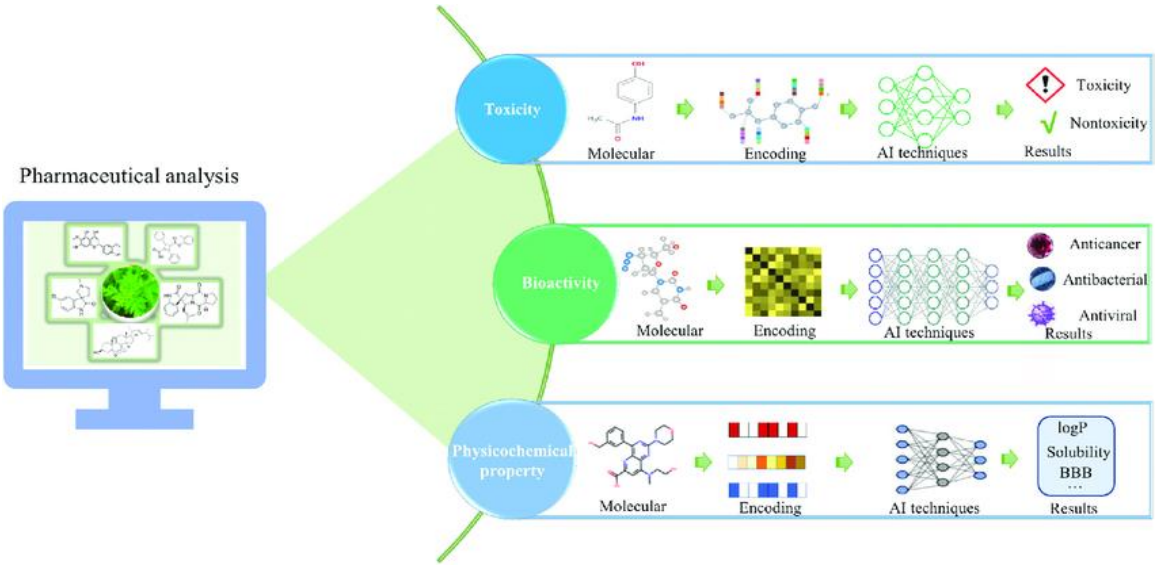

Figure 4. Application of AI techniques to pharmaceutical analysis.

Prediction of Physicochemical Properties

In the dynamic field of drug discovery, accurate prediction of the physicochemical properties of therapeutic candidates is important. AI has made a great impact in this area by providing effective solutions for determining properties, such as solubility, permeability, and stability. These are important for the drug to reach its intended purpose and increase its therapeutic effect. It is a resource-intensive and time-consuming process, which has led to the search for intelligence-based solutions. More importantly, the combination of neural networks using molecular annotations has been more effective, emphasizing the value of 2D molecular description in these analyses. The predictive power of AI extends to a variety of electrical properties, including distribution coefficient (logP), degree of ionization, and intrinsic permittivity, as well as resolution [116, 117]. AI-based tools leverage large datasets of previous compound optimizations to train models that can generate and predict valid molecules and their molecular descriptors, such as SMILES sequence, current capacity measurements, and electron density [10, 58]. Quantitative model-feature relationship workflows and neural networks have been developed to predict other important parameters, such as lipophilicity and acid dissociation constants, pointing to the use of fire electrical engineering in medicine. Various predictors were used to predict intestinal absorption of drugs based on parameters, such as molecular volume, logP, and solubility index, while CNN and unbiased neural networks were used to model solubility [61, 114–115].

In addition to solubility, the predictive power of AI extends to a variety of electrical properties, including distribution coefficient (logP), degree of ionization, and intrinsic permittivity. Role AI-based tools use large datasets of historical compounds to infer models that can be used to design and predict effective molecules and their properties. SMILES bands use molecular descriptors, such as potential energy and electron density [10, 58]. Quantitative structure a property relationship (QSPR) workflows and neural networks have been developed to predict other important properties, such as lipophilicity and acid dissociation constants, further demonstrating the utility of AI in drug development [10, 116–117]. For example, CNN and undirected RNNs were used to model solubility, while multiple predictors were used to predict the digestibility of compounds, such as molecular volume, logP, and solubility index [10, 118–119].

AI as contribution to drug product prediction extends to the rapid screening of drug candidates, identifying potential drug interactions, and assessing drug metabolism and toxicity. Advanced AI methods and predictive models for drug interactions, such as Image Mol, exemplify AI as an ability to improve and streamline the drug discovery process. These innovations provide a better understanding of behavior and interactions, enabling an easier path to drug development before clinical trials begin.

Drug Toxicity Prediction

AI has played a significant role in predicting drug toxicity and has made significant improvements in identifying adverse effects in new drug users. With careful study and application, AI models can be used to characterize toxicity by focusing on the cause of damage to the body or biological pathway. These features can be important in combining drugs with the least side effects, thus improving the selection of safer drugs [10, 58].

Toxicity is an important indicator of the danger of a substance and is also a major problem in drug development. In contrast, computationally driven cognitive processes are efficient and effective in predicting toxicity. They stand out for their accuracy in predicting toxicity [61, 120–122]. The use of AI in toxicity prediction is an important tool in reducing the risks associated with drug development. Tools like DeepTox are not only useful in chemical testing but can also help prevent adverse events early in the development process [18, 123] by helping to identify and resolve toxicological issues. Help monitor side effects, therapeutic targets, and safety before clinical trials begin. This is hoped to reduce the risk of failed trials due to unexpected toxicities, thereby improving drug safety and reducing post-marketing disruptions [18, 119, 123].

Furthermore, the use of AI to predict drug toxicity increases the efficiency in the assessment of chemical targets, genotoxicity, organ toxicity, cytotoxicity, and mitochondrial toxicity. High sensitivity of in vivo toxic effects. Quantitative structure–activity relationship (QSAR) models using a combination of methods, such as random forests (RFs) and SVMs show very good and robust results in predicting toxicity, outperforming traditional methods [18, 126–128].

Drug Bioactivity Prediction

The integration of AI into drug screening processes marks a transformative advancement in the field of drug discovery, particularly in the prediction of drug bioactivity. AI as a capability to uncover new targets through the identification of prospective interactions and the prediction of a compound as affinity for specific proteins or receptors is revolutionizing the way scientists assess the therapeutic potential and understand the mechanisms of action of drug candidates [10].

A major challenge in drug development is the assessment of biological activity, especially considering that many drugs of origin may not be effective due to the poor performance of biological organisms.

Experiment

Leveraging cost-effectiveness and efficiency, AI systems have become powerful tools for predicting drug activity, including antibiotics, pesticides, and antibiotics. New applications of AI in

predicting antimicrobial activity [61, 129] the model provides an easy way to find new disease drugs by generating molecular images from SMILES signals and extracting detailed information, assessing the pathogenic potential of molecules with high accuracy [7, 10, 61].

Drug–target association (DTBA) prediction is important for the evaluation of drug molecules a€™ efficacy. AI-based techniques make good use of both feature-based interactions that consider the properties of drugs and targets, and relationship-based interactions that assume that drugs with similar properties will interact with similar targets. Traditional tools, such as similarity analysis (SEA) and machine learning and deep learning, such as KronRLS, SimBoost, DeepDTA, and PADME were used to accurately predict DTBA. This cognitive process improves traditional methods by using advanced computational models that do not rely on the existence of 3D protein models, thus expanding the prediction process between drugs and protein targets [10, 130].

Deep learning models, such as DeepAffinity and PADME stand out with their ability to predict target interactions by combining drugs and targets. Gain a better understanding of DPI [131]. Additionally, AI-Â² application extends to the prediction of ADME (absorption, distribution, metabolism, and excretion) properties, which are important for understanding the pharmacokinetics of drug molecules. Tools, such as XenoSite and SMARTCyp help identify metabolic sites and specific isomers of CYP450 involved in drug metabolism, improving the prediction of drug elimination pathways and leading to a deeper understanding of drug metabolism [10,131–133].

Artificial Neural Networks

Artificial neural networks (ANN) are a significant technological advancement based on the neurophysiological structure of the human brain. One or more hidden layers transform the data from the relationship and the output layer where the final prediction or classification is made [134–138].

ANN consists of various types of networks, each designed for a specific application. Whether supervised or unsupervised, the simplicity of the training process and the ability to control reinforcement and feedback mechanisms characterize different ANNs [31, 139–140].

Historically, the use of neural networks has spanned many fields, from medicine and engineering to biology and pharmacology. They play a key role in enhancing drug delivery research. Their ability to interpret statistical models makes them invaluable in high-throughput virtual screening (HTVS), QSAR studies, and pharmacokinetic and pharmacodynamic modeling. The six stages of successful drug discovery are deeply rooted in important nonlinear relationships [6, 144–146].

In the context of drug research, the brain as connections has become a brain model that can solve the problem of inconsistency and disparity between standard layers. Their applications range from target-based and model-based drug discovery to the development of drug delivery systems, paving the way for new solutions and addressing the evolution of ANNs [134, 142].

RNNs

RNNs represent an advanced ANN specifically designed to process data connections, which makes them play an important role in fields, such as natural language processing, genomics, and especially drug research [135, 147]. Their looped architecture allows the network to store information from one step and pass it on to the next, facilitating the processing of variable-length input sequences. This capability allows RNNs to capture arbitrary physical behaviors necessary to analyze real-time data, genome sequences, protein structures, and Simplified Molecular Input Line Input System (SMILES) sequences [148].

However, traditional RNNs face problems in long-term learning on a dataset due to the gradient vanishing problem that affects the data stored on the continuum. These improvements include Long Short Chain-Term Memory (LSTM) networks and Gated Recurrent Units (GRU). These

improvements include a mechanism that chooses whether to store or discard data in a sequence [117] so that important values are retained for a long time without affecting the loss problem. This is what makes RNNs unique and useful. For example, RNNs are good at modeling protein–ligand interactions by identifying the relationship between amino acids in proteins and atoms in ligands; this is important for predicting the binding of drug molecules to proteins. Such predictions are important for evaluating the therapeutic potential of drug candidates [60, 149, 150].

RNNs are characterized by their unique design that incorporates feedback, which allows the network to use internal memory to process sequences. This architecture differs from feedback loops that allow the signal to loop back to the previous process for context and

CNNs

CNNs represent advances in AI, particularly in the processing and analysis of visual data. Spatial and hierarchical features make them very successful in identifying patterns in images. Through training, CNNs have demonstrated the ability to identify and analyze images from different sources [20, 117, 135, 151–153].

In drug discovery, CNNs have proven their effectiveness and efficiency, especially in predicting the biological activity of drugs, such as drug molecules. The molecular structure is represented as a 2D image. Each junction image encapsulates chemical elements, such as atoms and bond types, allowing CNNs to recognize complex patterns and predict chemical compounds based on a given target [78, 117].

Additionally, CNNs can learn representations directly from molecular models without the need for predefined models, which differentiates them from machine learning models. This difference simplifies the identification process [60, 154–155] by eliminating the traditional selection and reduction requirements.

CNN has also been successful in biological image processing due to its performance in computer vision. Their design includes convolutional and subsampling layers that effectively reduce the number of parameters, reduce memory requirements, and increase learning speed. This performance makes CNNs superior to other machines learning algorithms in image recognition and thus plays an important role in extracting useful information from biological data [60, 156]. Biological research areas include pharmacogenomics. This shift has become important in autonomous vehicles and precision medicine, where Ais, such as CNNs offer new solutions to medical problems. More importantly, CNNs have been used to analyze environmental biological information, such as nucleotide and protein abundances, driving advances in many biological sciences [157].

The use of new CNN architecture concepts, such as Siamese networks, continues to expand the application of CNN, from reuniting missing individuals with relatives to predicting drug interactions in drug research. Potential modifications including the prediction of ligand–protein interactions. CNN models have been useful for optimizing functional scores in ligand-protein studies by predicting the relationship and have shown their potential to increase predictive power in drug discovery [20, 158–162].

Feed-Forward Network

Feedforward neural networks (FNNs) represent the basic architecture in the ANN field and are characterized by a unidirectional data flow [60,163]. No loops or back-connections. This model forms the basis of FNNs; it is easy to use and can be applied to many applications, especially in drug discovery 164]. Radial basis function (RBF) networks, self-organizing maps (SOMs), and deep feedback. The choice of architecture depends on the requirements of the application; each variant provides unique benefits for pattern recognition, prediction, and data analysis [117, 164].

FNNs simulate biological processes and have a network of neurons, like computers or nodes, all of which contribute to the ability to make decisions in the network. Nodes process input data by performing heavy arithmetic operations to produce outputs that represent network predictions or distributions.

Female Gender

In drug research, FNNs are useful for modeling biological and drug interactions, supporting the identification of therapeutic targets, and optimizing drug users. Their computing power accelerates the path from experimental data to actionable insights, affecting the speed and accuracy of treatment [165].

Multilayer Perceptron

The multilayer perception (MLP) is the basis of the ANN architecture and is characterized by a transmission model where data are processed by an input process and one or more hidden processes at the output [140]. The combination of good knowledge in academic supervision makes it very useful, especially in pharmaceutical research [31].

Essentially, MLPs are a variation of FNNs designed to teach the process of accessing common objects. They are trained using a back propagation algorithm that allows the elbow in the network to be adjusted according to the error between the actual output and the desired output. This error correction allows the MLP to adjust its prediction so that the prediction is accurate in time. The structure of this network is like a map, where the connections and weights help to adjust according to the errors present in the output nodes, thus improving the performance of the network to predict complex patterns and relationships in the data [20]. Or do a dynamic like logistic sigmoid [6, 166] as a function of poor performance in modeling. The transformation of MLPs to CNNs is a significant change that allows many MLPs to be connected in sequence, strengthening their measurement capabilities [6, 167–168].

In the context of predictive modeling in ANNs, MLP is a powerful tool for data analysis. MLP usually has three main layers: input layer, overlay layer, and output layer. Each of these layers contains neurons connected by weights, with additional parameters that determine the threshold for neuron activity. Benefits of non-essential processes, including drug discovery and development. The application of MLP continues to model biogas treatment processes, where parameters, such as influent pollutant concentration and gas concentration are crucial. MLP demonstrates its versatility in designing models that can predict human elimination by leveraging insights from bioprocess research [169].

AI-Based Tools in Drug Discovery

The advent of AI technology will change the meaning of drug discovery by allowing researchers to analyze large data sets, develop molecular models, and predict the performance of potential drug candidates [29].

AlphaFold

The revolutionary AI tool AlphaFold is based on DNN and has made significant progress in predicting 3D protein structures.

Progress

AlphaFold demonstrated its ability to successfully predict protein structures by correctly predicting 25 out of 43 protein structures [10, 29, 61, 170–173].

AlphaFold evolved into its next version, AlphaFold2, with faster and more accurate protein structure predictions. However, translating these predictions to in vivo conditions remains challenging. AlphaFold2 was specifically trained to predict the structure of disordered proteins; many

drug discoveries require information about protein-small molecule complexes. Furthermore, achieving the sub-angstrom resolution often required for drug design is still beyond AlphaFold2 as capabilities. However, [29,172] AlphaFold as capabilities shine in the production of therapeutic proteins, such as antibodies and peptides, where ultrahigh resolution is not a prerequisite. Understanding the relationship between protein structure and function has become essential (Table 2). By solving protein structure and detecting damaged proteins, AlphaFold helps us to understand many diseases, accelerate drug development, and combat pandemics [28–29].

Table 2. List of AI-based software for drug discovery [10].

Tools	Details	Website URL	References
DeepNeuralNetQSAR	Python-based system driven by computational tools that aid detection of the molecular activity of compounds.	https://github.com/Merck/DeepNeuralNet-QSAR	[183]
DeepChem	MLP model that uses a Python-based AI system to find a suitable candidate in drug discovery.	https://github.com/deepchem/deepchem	[184]
ORGANIC	A molecular generation tool that helps to create molecules with desired properties. https://github.com/aspuru-guzik-group/ORGANIC	https://github.com/aspuru-guzik-group/ORGANIC	[185]
PotentialNet	Uses NNs to predict binding affinity of ligands. https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	[109]
Hit Dexter	ML technique to predict molecules that might respond to biochemical assays. hitdexter2.zbh.uni-hamburg.de/	http://hitdexter2.zbh.uni-hamburg.de	[10]
DeltaVina	A scoring function for rescoring drug–ligand binding affinity. https://github.com/chengwang88/deltavina	https://github.com/chengwang88/deltavina	[10]
Neural graph fingerprint	Helps to predict properties of novel molecules. https://github.com/HIPS/neural-fingerprint	https://github.com/HIPS/neural-fingerprint	[10]
DeepTox	Software that predicts the toxicity of total of 12 000 drugs. www.bioinf.jku.at/research/DeepTox	www.bioinf.jku.at/research/DeepTox	[186]
AlphaFold	Predicts 3D structures of proteins. https://deepmind.com/blog/alphafold	https://deepmind.com/blog/alphafold	[10]
Chemputer	Helps to report procedure for chemical synthesis in standardized format. https://zenodo.org/record/1481731	https://zenodo.org/record/1481731	[10]

IBM Watson

IBM Watson is a key element in the development of intelligence and has a model designed to provide correct answers from structured and unstructured data [6, 174], which has achieved great success with its ability to process good words. A person who has gained international recognition. This success is supported by DeepQA, an advanced language processing system developed by IBM that allows Watson to understand questions in detail and produce correct answers. The investigation produced many answers by collecting evidence from many sources. These answers were evaluated during training using multilevel logistic regression, and the most meaningful answers were rigorously tested to determine the most correct [6].

While the campaign raises hopes for Watson as a revolutionary approach to healthcare, its contributions are significant. Watson helps oncologists recommend personalized cancer treatment plans by analyzing patient information and medical records. It also helps interpret medical images, increasing the accuracy of radiography, and thus improving the detection of abnormalities [6, 175].

DeepChem

DeepChem is an open-source deep learning platform specifically designed to facilitate the use of AI technologies in drug discovery and chemoinformatics [33, 176] projects. Many aspects of research and chemoinformatics studies benefit from deep learning [134]. One of the key features of DeepChem is the MoleculeNet dataset, which contains resources for over 700,000 compounds and is a key resource for training and applying deep learning models in drug discovery and research projects [177].

Importantly, DeepChem as capabilities extend beyond academic research as it is adopted from industry, including formulation, hardware, and evaluation, to commercial drug [176, 178] development and guiding ligand screening for commercial drugs. Use the computing power of NVIDIA GPUs to accelerate computation and improve the performance of deep learning models in drug discovery [33, 179]. Potential methods and tools to apply deep learning models to all aspects of drug discovery and development

DeepTox

DeepTox is a software specifically designed to predict the potential toxicity of various drugs. The ability to measure many drugs simultaneously makes it an important part of the important process of drug safety assessment. DeepTox uses the power of deep learning, a type of machine learning that specializes in processing complex, multi-layered data. This allows DeepTox to learn and predict a wide range of potential chemicals in a single neural network, ultimately providing drug labeling information. A DeepTox pipeline first normalizes the drug representation of the drug being analyzed. A set of chemical descriptors is then calculated and fed into the machine learning algorithm. Through an iterative process of training, analysis, and integration, DeepTox combines best practices to create a powerful product. Finally, DeepTox provides toxicity predictions for new compounds, allowing researchers to assess risks associated with drug candidates during drug discovery and development. The tool is publicly available at www.bioinf.jku.at/research/DeepTox and enables researchers worldwide to leverage its potential to improve drug safety and reduce adverse reactions [33, 61, 122].

ORGANIC

ORGANIC (Generation Augmented Generative Adversarial Networks for Reverse Engineering Chemistry) is a powerful design tool that helps scientists create molecules with desired properties. GANs and RL. The GAN component is responsible for the production of non-repetitive, precise molecular species, while the RL component influences the distribution of specific products, ensuring that molecules are produced according to the required pattern. ORGANIC is particularly important in the early stages of drug discovery, where the creation of new drugs with specific therapeutic properties is a key step. Molecules with therapeutic properties. at The ORGANIC framework is publicly available and accessible from the project as GitHub repository (https://github.com/aspuru-guzik-group/ORGANIC), allowing researchers from around the world to work on the drugs they discover. This open approach encourages collaboration and enables the development of new treatments, ultimately benefiting the broader research community and ultimately improving patient outcomes [33, 71, 180].

Hit Dexter

Hit Dexter is a machine learning program designed to identify hit associations. The development methodology uses various machine learning methods, including Random Trees (ETC), RF, AdaBoost, and Bagging classifiers. The values range from 0.56 to 0.58. External validation shows that the best model can identify the correct uncorrelated MCC value up to 0.64 and the area under the receiver operating characteristic curve (AUROC) value up to 0.96. One of the main benefits of Hit Dexter is its ability to predict the variability of currently sold drugs. The sample determined that approximately 13% of the pharmaceutical market is impure drugs, of which 6% are classified as substandard. In addition, this web server offers a variety of chemical sites, including dark drugs, polymerization drugs, high-throughput screening (HTS) drugs, drug-like drugs, drug interaction effects (PAINS), and

natural products. Hit Dexter provides online access (http://hitdexter2.zbh.uni-hamburg.de) allowing users to access the integrated ML model and code to identify the right types of people and methods that could harm drug research [181–186].

Instance-Based Methods

Example-based methods, often referred to as memory-based methods, belong to the category of a lazy learning algorithm. These methods, which include nearest neighbor (KNN) and case-by-case (CBR) methods, are widely used in many areas, such as pattern recognition, classification, and backward working. Search large libraries to identify molecules with similar structures or activities to known drugs or drug targets [117, 187, 190].

K-Nearest Neighbors (KNNs)

The KNN algorithm stands out with its results in big data mining and drug discovery. Conceptually, compounds are planned in a multidimensional space and each dimension represents a narrator. The predefined K-value is reported as the square root of all compounds in the dataset. For example, for 400 compounds, K is approximately [20, 191–197].

By identifying the properties and biological functions of neighbors, KNN can use similar methods (e.g., chemical substances with similar structures and biological functions of similar individuals) to facilitate the prediction of the clinical, toxicity, or pharmacokinetics of new drugs. KNN as drug discovery program allows researchers to use the existing rich database of known compounds to rapidly screen and screen potential drug candidates. A data-driven approach can accelerate the early stages of drug discovery by identifying high-quality crystals and optimizing their properties before moving to resource testing and clinical trials.

Case-Based Reasoning (CBR)

CBR is an AI method that solves new problems by reusing solutions from similar past situations. The CBR system has a data library that collects problem-solving documents, each containing a problem description and solution. When a new problem [198–200] arises, CBR searches the library for similar past cases based on similar metrics. Solutions from similar situations are often adapted or reused to solve new problems. A CBR has proven particularly useful in problem-solving and health promotion decisions for several important reasons. History taking is an important part of clinical training, and the literature is enriched with narratives describing individual treatment. Even if there are methods, they should be explained and supported and in the study with background information found in examples, even hello. Reasoning by example is based on the intellectual process of doctors. Evidence in general, the use of CBR is based on clinical knowledge, the complexity of biological diseases, and the harmony with the thought process of doctors [201].

Decision Tree Algorithms

A decision tree algorithm is a model that uses a tree structure to represent a decision based on certain characteristics or predicted values of the input data. They are usually used for classification or prediction. This classification continues by splitting the data into more and more processes with binary decisions until the final decision or end of flight is reached. Ideally, each terminal will represent a data point and its label, but the splitting process will stop before it gets too large to avoid over fitting and increase the capacity of the model [202].

However, decision tree models can have some limitations. One of the main problems with decision tree algorithms is that they tend to overshoot due to their high variance. This means that they can detect noise or irrelevant patterns in the data [202]. On the other hand, they can also introduce bias by simplifying relationships in the data. A RF is a collection of decision trees where each tree is trained on a different starting dataset [203]. A pharmaceutical companies use decision tree algorithms at various stages of drug discovery to help identify and develop new drugs. Before the ingredients are mixed [117, 204].

AI in Clinical Trial Design

Designing a clinical trial is an important part of bringing a new drug to the market, including determining the conditions needed to achieve significant results. This step is important in estimating the incidence in the target population, calculating the expected number of patients, and calculating the follow-up period needed to calculate the expected incidence. During this study, patients were closely monitored until a predetermined number of events were achieved. A successful drug development process [29, 205–206] will take 10–15 years to complete and will cost between $15 and $2 billion (Figure 5).

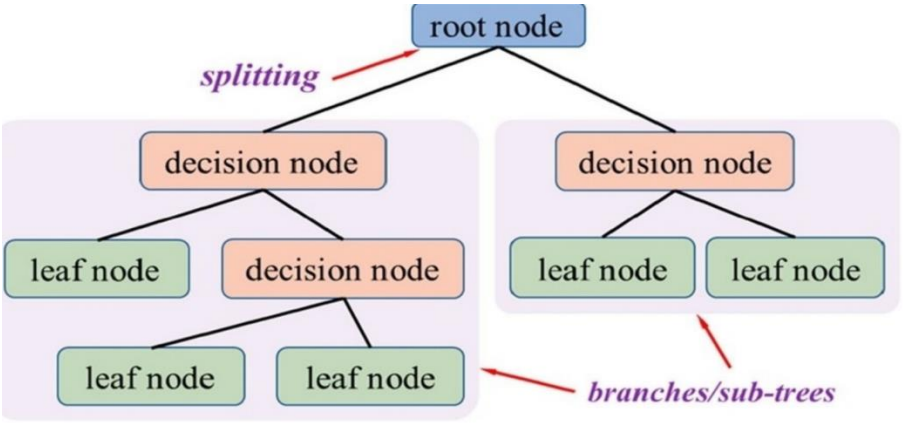

Figure 5. Schematic diagram of the decision tree [117].

Most of the time and investment goes to clinical trials, which take 6–7 years and require significant financial investment in disease conditions. However, the success rate is dubious, only one in 10 molecules that enter clinical trials is successfully licensed, causing a huge loss to the industry. These failures can be caused by many factors, such as poor patient selection, insufficient requirements, and weak systems [10, 207].

The remaining 50% of R&D expenditure is allocated to preliminary activities, which include discovery, pre-testing, and regulatory processes. Appropriate patient selection is difficult because inappropriate patient selection leads to approximately 86% failures. Optimize the clinical trial process to shorten time to market and reduce associated costs. Due to the availability of large amounts of digital medical information, the use of AI has emerged as a promising option; providing the ability to change all aspects of clinical trials and practices, ultimately accelerating the development and implementation of new treatments [10, 29, 208–210].

AI algorithms can rapidly evaluate thousands of compounds by simulating the interactions between drug molecules and biological targets, thus reducing the time and resources required for early drug discovery. Simulations of biomolecular structures using physically based atomistic methods, such as molecular dynamics (MDs) [211]. Model-predicted 3D structures of proteins and drugs. This technique provides a long-term view of atomic motion by examining the stability, dynamics, geometry, and functional connectivity of protein–drug complexes. Advanced data analysis techniques, including deep learning, can then be used to analyze these systems and gain new insights into patterns of change and interaction in biological processes. This knowledge can help resolve questions about diseases, pathways [171, 212] and mechanisms of drug response or resistance capacity. This approach accelerates early drug discovery and facilitates the identification of drug candidates [213].

Challenges and Limitations of AI in Drug Discovery

Although AI holds great promise to revolutionize drug discovery, there are still challenges that need to be addressed to realize its full potential. A key challenge is ensuring data quality and

availability. Intelligence models are data-driven, and their effectiveness depends on the amount and variety of data they learn. Good biometric data are difficult to obtain due to privacy laws and data segregation among schools. Furthermore, generating the necessary data can be expensive and time-consuming, especially for small research groups. Collaboration and knowledge-sharing initiatives therefore play an important role in ensuring access to a wide and diverse range of information [214–215].

There are also significant limitations to misinformation and generalization. AI models can produce incorrect predictions when trained on biased data. These biases can arise from underestimating the specific population in clinical trials, geographic differences in the data, or differences between physicians. Furthermore, over fitting is characterized by a model that performs well with training data but is difficult to process with unobserved data, which can lead to misidentification of drug users or [216–217] negative outcomes. At this stage, bias correction technology is used to reduce the effect of bias on the output model. For example, in cognitive-behavioral research, the use of [218] SMOTE (Synthetic Minority Oversampling Technique) bias corrections can solve the problem of data bias. Dispersion Methods to correct for bias have been explored, but there is no universal solution yet. However, through careful data selection, processing, and bias correction procedures, researchers can reduce the impact of data bias on AI application forms.

Processing power and resource intensity are also significant challenges, especially for deep learning models. These models require substantial computational resources for both training and inference, posing barriers for smaller pharmaceutical companies and academic research teams with limited budgets. Cloud-based AI services and collaborations with AI technology providers are being utilized to reduce computational costs and enhance accessibility. Moreover, regulatory approval and validation are critical aspects that AI models in drug discovery must undergo. Demonstrating the safety, effectiveness, and repeatability of AI-generated outcomes is essential for gaining regulatory clearance and building confidence within the pharmaceutical sector. Collaboration among regulatory authorities, pharmaceutical companies, and AI researchers is crucial for establishing validation procedures and guidelines [219].

Cost considerations are also important, as significant investments in technology, data collection, and technology personnel are required. Solving these financial challenges requires a long-term perspective while exploring government incentives, effective partnerships, and financial collaboration models [220].

CONCLUSIONS

The integration of AI in drug development and discovery is important for the pharmaceutical industry, which has a significant impact on improving the quality and efficiency of medical services. AI not only accelerates the drug discovery process through many applications, but also opens up new avenues for drug repurposing, target identification, and prediction of new drug use. The important role of AI in repurposing expands its ability to replace traditional drugs, making it an important tool in the search for new treatments. The use of AI in drug analysis and analysis shows the potential to improve drug development. Scientists can use the computational power of AI to identify and isolate targets, thereby evaluating drug candidates. This computational efficiency extends to polypharmacology, drug synthesis, and drug repurposing, suggesting the evolution of AI to improve global health outcomes.

The emergence of machine learning, an important part of AI, has strengthened the field of drug discovery by developing models that can learn and make predictions. Networks, such as MLPs, RNNs, CNNs, and FFNs play a significant role in processing complex data, improving accuracy and reliability in drug development. New AI systems and software, such as IBM Watson, DeepChem, DeepTox, ORGANIC, and Hit Dexter are highlighting the diversity of tools available to support drug discovery. Methods, such as KNN, CBR, and Decision Tree Algorithms are examples of various AI techniques that help in identifying potential candidate competition and developing quality

pharmaceutical products. However, despite these advances, AI also faces challenges in drug discovery. Misinformation, return on investment issues, limitations in understanding drug use, compliance with current procedures, and business changes are still alarming issues. Solving these challenges will require researchers, industry stakeholders, and regulators to work together to unlock the full potential of AI while minimizing its limited impact. Ultimately, AI as a contribution to the advancement of medicine is significant, giving way to more effective, efficient, and personalized medicine. As the pharmaceutical industry continues to embrace AI, overcoming the inherent challenges is essential to realizing the full potential of AI and ultimately advancing medicine and medical research.

What About India?

Developing new AI tools for drug discovery requires the use of large-scale hardware, especially high-speed processing units (GPUs), to work on multiple tasks for longer periods of time. GPU chips are expensive and become obsolete quickly as hardware manufacturers churn out new, faster GPU chips every year. India needs such a large enterprise in the economy. This, along with the lack of AI researchers, is the second reason why Indian researchers have not been able to achieve the best results in developing AI tools for medical design, despite having expertise in proteins, unlike the US and China. The rich history of X-ray crystallography, structure, and other biology studies. But as the number of medical institutions continues to grow, India can take the lead in using AI to focus on detection, analysis, and drug testing.

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