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Role of Artificial Intelligence in Drug Discovery

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Abstract

Traditional drug discovery methods, such as synthesis operations, validations, and testing in a wet laboratory, are time-consuming and expensive. The use of artificial intelligence (AI) methods in the pharmaceutical industry has been transformed by recent developments in the field. Artificial intelligence methods, when coupled with easily available data resources, are altering the course of medication development. For different phases of drug development, a number of AI-based models have been created in the last few decades. By supplementing traditional trials, these models have hastened the process of drug discovery. Molecular representation techniques are used to transform data into representations that computers can understand. We began by outlining the most popular drug discovery data sites, including ChEMBL and DrugBank. At the same time, we compiled a list of all the algorithms that went into creating AI models for medication development. We then moved on to talk about how artificial intelligence (AI) methods may be used in pharmaceutical research to forecast things like a drug's physicochemical properties, bioactivity, and toxicity. In addition, we presented the AI-powered models for creating new drugs, predicting their structures and interactions with targets, and determining their binding affinities. We went on to mention AI's cutting-edge uses in nanomedicine design and drug synergism/antagonism prediction. Lastly, we covered the benefits, drawbacks, and potential future directions of artificial intelligence in the pharmaceutical industry.

Keywords: Artificial intelligences, drug discovery, de-novo drug design, nanorobots, deep learning

Introduction

Drug discovery refers to the process of finding new medications to cure illnesses. An abundance of specialized expertise and technology resources are required. A new treatment typically takes around fifteen years and $2.8 billion to be discovered. Traditional methods, with their high costs and low efficiency, have become roadblocks in the drug development process. Therefore, we need figure out more efficient methods to deal with this tedious and expensive task.

Now that multi-omics data is readily available and high-performance computing has progressed, AI methods are finding real-world uses in many different industries. When it comes to analysing biological data in particular, the pharmaceutical industry has seen the efficient application of AI tools. So far, AI techniques have been used in drug discovery operations for a variety of purposes, including drug-target prediction, bioavailability, and de novo drug design.5 The pharmaceutical industry has begun to collaborate with IT companies in an effort to develop drug creation methods grounded in artificial intelligence approaches. Pfizer, Bayer, and Roche are among these corporations. The Insilico Medicine team just used AI to discover a treatment for idiopathic pulmonary fibrosis. The therapy has shown promising results in phase I investigations. Thus, it is acceptable to claim that the pharmaceutical sector has entered a new age due to AI.

In this article, we will go over the fundamentals of using AI methods for drug assessment and development. Collecting data, curating compound representations, and using AI algorithms for drug development are the main approaches. We began by presenting researchers to representative data resources, molecular representations and descriptors, and AI techniques in drug discovery so that they could get a catch-up picture of the advancement in this area. We continued by outlining the many phases of drug development and how AI has been successfully used to each. Lastly, we went over some of the obstacles and potential solutions to using AI in

drug development in the future.

The creation of new medications may be accelerated and kept down in cost with the use of artificial intelligence, which has several practical applications including language modelling and pharmaceutical industry improvement. Experts in the field of drug development confront the challenge of creating a method for administering therapeutic chemicals to their target that is both effective and safe. It takes a lot of effort and money to create new pharmacological molecules. What we call "drug discovery" is really the process of identifying new medications to cure illnesses. Modern developments in high-performance computing and the availability of multi-data sets have paved the way for AI approaches.

Machine intelligence, or artificial intelligence (AI), is the practice of teaching computers to think and solve problems in the same way as humans do. This is a simulation of human intellect.1 Artificial intelligence (AI), covering possible methods, applications, and fundamental challenges. As a first step, let's take a high-level look at artificial intelligence (AI) and all its subfields, such as deep learning (DL), machine learning (ML), etc. 2 Innovation in the pharmaceutical sector usually stems from extensive research and development in several domains, including as manufacturing technology, packaging issues, and customer-focused marketing strategies. New pharmacological advances include biologics and small molecule medicines. To satisfy unmet demands in illness therapy, it is recommended that medications have better stability and high potency. Data augmentation and explainable AI (XAI) are two potential solutions that they look at. They also discuss some of the practical obstacles with AI being used in drug development, such as data availability, ethical concerns, and combining AI with traditional methods.2 Unlike conventional medication research, which takes five years, artificial intelligence medicine only takes twelve months to reach the trial stage. The exponential growth of the life sciences and machine learning has yielded a wealth of data information on the current upsurge in AI-driven drug discovery enterprises. In Figure 1.

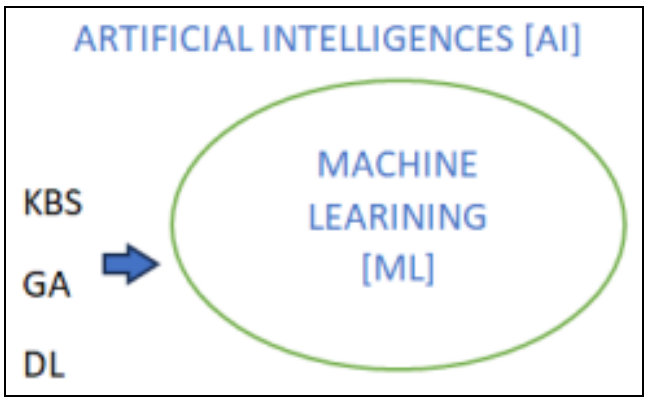

Fig 1: Artificial intelligence in drug discovery [AIDD]

Literature Review

Artificial intelligence (AI) refers to the modelling of human behaviour in relation to the intellectual processes involved in problem solving. Some examples of these processes in action are reading, observing, planning, interpreting, reasoning, correcting, voice recognition, linguistics, and human cognitive science. By teaching computers to learn from mistakes and fix them, adapt to new and random input values, learn from their own experiences, and do human-like tasks with ease via thorough scenario analysis, artificial intelligence (AI) simplifies operations. Artificial intelligence (AI) simplifies tasks by analysing, filtering, sorting, predicting, and figuring out large amounts of data in accordance with best practices for implementing solutions. The pharmaceutical industry is currently utilising AI primarily for the following purposes: drug discovery and development; drug-adherence and dosage; improving analytics by making sense of clinical data; finding more reliable patients for clinical trials more quickly; introducing automated robot pharmacies to fill prescriptions and dispensing; and marketing, logistics, and supply chain. These applications were last updated in 2019. Most importantly, AI has the ability to save lives via the creation of innovative, cost-effective therapies and the reduction of associated expenditures. To that end, biotech companies should get on the AI bandwagon. Machine learning and artificial intelligence solutions will therefore be very beneficial to the industry. It has the potential to be used to construct a strong and sustainable pipeline of new pharmaceuticals. If we could tap into the capabilities of modern supercomputers and machine learning, we could speed up and reduce the cost of medicine development. This study examines the current situation of AI in pharmaceutical sciences, particularly as it pertains to the pharmaceutical business. Finally, as technology advances, human healthcare experts will also have to grow, learn, and adapt; human-machine collaboration is the wave of the future. Although future specialists will need expertise in both medicine and technology, this does not mean that medicine is becoming extinct; rather, it is undergoing a period of evolution.

Blanco-Gonzalez, Alexandre & Cabezon, Alfonso & Seco-Gonzalez, Alejandro & Conde-Torres, Daniel & Antelo-Riveiro, Paula & Piñeiro, Ángel & Garcia-Fandino, Rebeca. (2022) [1]. The use of artificial intelligence (AI) might significantly enhance the drug development process by providing faster, more accurate, and more efficient results. On the other hand, AI can only be useful if high-quality data is readily available, ethical issues are addressed, and the limits of AI-based systems are acknowledged. Here we take a look at the pros, cons, and overall state of artificial intelligence (AI) in this industry, and we provide some solutions to the problems we see. We also talk about the possible benefits of AI in pharmaceutical research, how to employ explainable AI, data augmentation, and how to combine AI with conventional experimental approaches. Taken as a whole, this analysis sheds light on the possibilities of AI in the drug development process and offers advice on how to overcome obstacles and seize opportunities. Important message from the authors: Our goal in generating this post was to see how well ChatGPT, a chatbot trained on the GPT-3.5 language model, could work with human writers to produce review pieces. We tested the AI's capacity to autonomously produce material using the text it produced after we provided it with instructions (see to the supporting information for details). Following a comprehensive evaluation, human writers essentially rewrote the paper, aiming to strike a compromise between the initial concept and scientific standards. Using AI for this

purpose has both benefits and limits, as stated in the previous section.

The integration of AI into drug development signifies a watershed moment in pharmaceutical research, combining advanced computational methods with traditional scientific investigation to overcome long-standing hurdles. This article provides a comprehensive overview of the many ways AI is being used in the drug development process, including recent innovations and new approaches. It explores how artificial intelligence (AI) is helping with drug design, poly pharmacology, chemical synthesis, repurposing drugs, and predicting physicochemical, toxicological, and bioactivity aspects of drugs. This study discusses the data quality, generalizability, computing needs, and ethical problems that have been faced in the area of artificial intelligence, in addition to the hopeful improvements that AI has made. This article provides a thorough review of artificial intelligence's function in the pharmaceutical industry, highlighting the technology's ability to greatly improve drug development while also recognizing the challenges that need to be solved to completely experience its advantages.

Liebman, Michael. (2022) [2]. The area of artificial intelligence (AI) is dynamic and promising. Artificial intelligence (AI) techniques are necessary for the thorough examination of data-related information because of the large and ever-increasing amounts of data. The use of artificial intelligence (AI) has grown in significance within the drug discovery and development industry as a whole, particularly in the areas of medicinal chemistry, formulation development, toxicology, pharmacology, pharmacokinetics, molecular and cell biology, upscaling, and medicinal chemistry. Clinical trials may greatly benefit from AI's ability to improve trial design (biomarkers, effectiveness parameters, dosage selection, trial length), target patient population selection, patient stratification, sample assessment, and overall success rate. There are an increasing number of start-ups focused on artificial intelligence (AI) for drug discovery and development, more and more partnerships between pharma and AI platforms, and a deluge of articles and reviews detailing AI's present uses, successes, and failures in this space.

Paul, Debleena & Sanap, Gaurav & Shenoy, Snehal & Kalyane, Dnyaneshwar & Kalia, Kiran & Tekade, Rakesh. (2020) [3]. The pharmaceutical business is one of the first to reap the benefits of artificial intelligence (AI), which has just lately begun to expand its use across many parts of society. Drug repurposing, clinical trials, drug discovery and development, pharmaceutical productivity, etc. are just a few of the many areas that have benefited greatly from AI, which has reduced human workload and increased efficiency in the pharmaceutical industry. Also covered are the methods and resources used to enforce AI, the problems that have arisen thus far, potential solutions, and the trajectory of AI within the pharmaceutical sector moving forward.

AI in the Drug Screening

Extraction of medicinal compounds from natural sources or mechanical processes used to be the primary means of drug discovery in the past. Regulatory approval and six Phase II clinical trials for pharmaceutical substances were failed. Algorithms such as RF, SVMs, DNNs, RF-Nearest-The classifiers, and extreme learning machines are used for VS, depending on the synthesis feasibility. Furthermore, these algorithms are capable of assuming *in vivo* activity and toxicity. It is important to take intrinsic permeability into account while creating novel medications, along with other physicochemical properties as the drug's solubility, ionisation degree, and partition coefficient (log P). The creation of organic substances and the use of identification methods like as mass spectrometry, gas chromatography-mass spectrometry (GC-MS), nuclear magnetic resonance (NMR), and high-performance liquid chromatography (HPLC) were among the first domains where the paradigm of discovery emerged. In the 1980s, rational drug design and structure-based drug discovery methods, as opposed to "random searches," became more prominent in the field of drug design as a result of technological breakthroughs in crystallography and computers. Online chemical testing and refinement, protein-drug interaction prediction, and molecule bioactivity assessment are all areas that might benefit from the use of artificial intelligence (AI). With the use of AI, virtual screening may improve by creating prediction models that choose compounds with a good likelihood of binding to a target protein.

Application of AI to pharmaceutical analysis

Pharmaceutical analysis is a crucial step in the drug development process that includes identifying, determining, quantifying, and purifying pharmaceutical raw materials. When it comes to pharmaceutical research, qualitative and quantitative analytics are king. Despite the excellent accuracy of these methods, they are still too costly to screen a large number of natural compounds for potential new drugs. Computational methods incur astronomically low costs as compared to experimental approaches. Thus, artificial intelligence methods have been integrated with experimental methods to enhance pharmaceutical analysis.

Drug toxicity prediction

A chemical's toxicity level indicates the degree to which it causes undesirable side effects. Finding chemicals with negative effects on people is the goal of toxicity assessment, a crucial stage in the drug discovery process. Drug development becomes more expensive due to the *in vivo* test's reliance on animal testing. The benefits of computational approaches include the ability to efficiently and cheaply anticipate a chemical's toxicity. To that end, a number of approaches based on AI techniques have been created to forecast chemical toxicity. The scientific community set up the "Toxicology in the 21st Century (Tox21)" challenge to evaluate various computer tools' abilities to forecast compounds' toxicity.

The core architecture of DeepTox, an ensemble model for chemical toxicity prediction, is a three-layer deep neural network (DNN). The remaining compounds are encoded using the above 0D to 3D molecular descriptors, which are fed to DNN, after data cleaning and quality check. The optimization and tweaking of a collection of hyperparameters-including the number of hidden units, learning rate, and dropout rate-provides the DeepTox pipeline. When compared to other methods for toxicity prediction using the Tox21 dataset, DeepTox comes out on top.

Drug bioactivity prediction

Actually, a lot of natural product-derived medications don't work since they don't have any bioactivity. Because of this, evaluating the bioactivity of drugs is a hot topic in the pharmaceutical industry. It is still costly and time-consuming to conduct *in vitro* and *in vivo* tests, even if they can simulate molecular activities in the human body. Anticancer, antiviral, and antibacterial medication bioactivities have been efficiently predicted using AI methods due to their time and cost savings.

For instance, a directed message passing neural network that may predict antimicrobial activity was suggested by Stokes *et al*. A molecular graph was initially built for each molecule using its SMILES, and the feature vector was derived using atomic properties (such as atomic number and number of bonds) and bond information (such as bond type and stereochemistry). The optimised feature vector was input into the feedforward neural network, which then produced the antibacterial likelihood of a chemical, by repeatedly executing the message passing process.

Drug physicochemical property prediction

Medicines have inherent qualities known as physicochemical properties. To comprehend and simulate the effects of medications, one must be knowledgeable about their physicochemical characteristics. Solubility is a crucial physicochemical property as it influences pharmacokinetics and medication formulations, among many others. Nevertheless, quick solubility prediction has been hindered by expensive and time-consuming experimental methods; hence, a lot of work has gone into developing AI-based solubility prediction models.

Panapitiya *et al*. evaluated several deep learning algorithms and molecular representation approaches for solubility prediction. These methods included fully connected neural networks, RNNs, graph neural networks, and SchNet. Molecular graphs, molecular descriptors, SMILES, and 3D atomic coordinates were also considered.54 The scientists discovered that the fully connected neural network outperformed the others when it came to solubility prediction using chemical descriptions, using the identical test dataset. Further analysis by the authors revealed that 2D molecular descriptors contributed the most to prediction when compared to other variables.

De novo drug design

In de novo drug design, a beginning template is not used to generate unique drug-like molecules. Despite their usefulness in the past, traditional structure-based and ligand-based drug design approaches have limitations when applied to contemporary drug discovery. These approaches depend on specific information about the biological target's active site or the pharmacophores of an existing active binder, respectively, which limits their ability to uncover small-molecule drug candidates. With the proliferation of AI techniques, the drug discovery process has been sped up and new possibilities for de novo drug creation have emerged.

There have been many proposals for deep learning-based models for de novo drug creation in recent years. These include ReLeaSE, ChemVAE, GraphINVENT, MolRNN, and ReAINN, among others. Molecular modelling is an additional cornerstone of new medication development. Algorithms for deep learning have used SMILES, fingerprints, chemical graphs, and three-dimensional geometries as input. On the left-hand side of the screen, you can see the basic structure of de novo drug creation approaches that rely on deep learning.

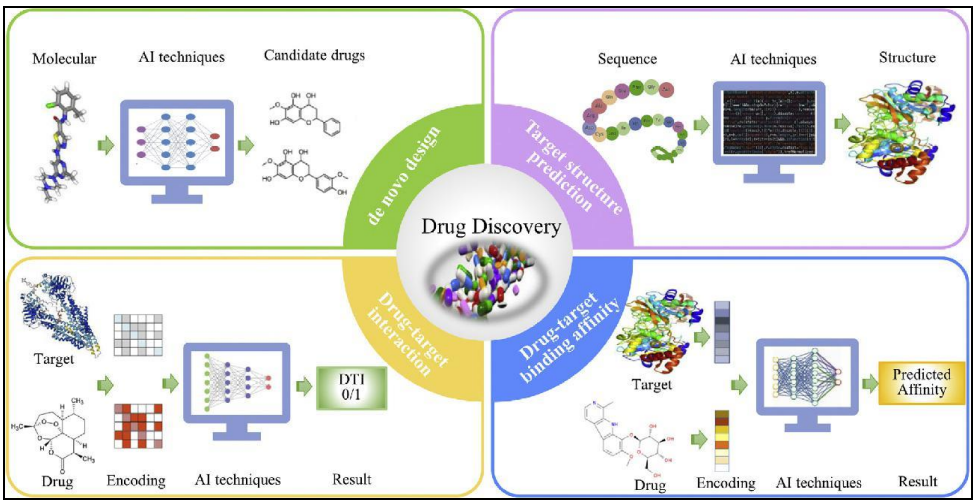

Fig 2: AI techniques for natural product-inspired drug discovery

Target structure prediction

Proteins involved in enzymatic activity, cell signaling, and cell-cell transmission represent the majority of pharmacological targets. A protein's shape dictates its function. Traditional experimental methods for protein structure determination, including X-ray crystallography, cryogenic electron microscopy, and nuclear magnetic resonance spectroscopy, are still labor-intensive and expensive. As previously stated, the structures of only 100,000 distinct proteins have been decoded using experimental methods. This represents a minuscule fraction of all proteins now known. Due to the large gap between the amount of protein sequences and the number of protein structures known, there is an immediate need to create new approaches.

Protein structure prediction has seen a proliferation of computer methodologies, thanks to advances in AI and the exponential rise in computing power. To the right of the top

right corner are the computational protein structure prediction models' fundamental schematics. The top-performing technique is DeepMind's AlphaFold, which uses neural networks to get accuracies comparable to those of tests in predicting the three-dimensional structures of proteins from their amino acid sequences. In Senior *et al*., we get details on AlphaFold's design and algorithm.

DTI prediction

Interactions between chemical compounds and their biological targets, such as proteins, are the subject of DTI prediction. One of the most important steps in developing new drugs is DTI prediction. Therefore, DTI has been determined experimentally using techniques like yeast two-hybrid, phage display technology, and co-immunoprecipitation. Predicting DTI using these wet laboratory methods, however, is a laborious process. More and more biological data has recently made it possible to predict DTI in silico. Consequently, DTI prediction is increasingly relying on computational approaches. As outlined in a recent study, these approaches may be grouped into five types: ligand-based, docking simulations, gene ontology-based, text mining-based, and network-based.

In many cases, deep learning-based algorithms outperform other kinds of methods when it comes to DTI prediction. In the lower left corner is a picture of the typical process flow for DTI prediction methods that use deep learning. The first step in the encoding process is the identification of relevant characteristics of chemicals and proteins. The next step is to feed the deep learning algorithms the chemical and protein feature embeddings. This approach has led to the proposal of drug-protein interaction prediction models based on CNN, multiple layer perceptrons, and deep belief neural networks, which has greatly accelerated the process of drug development.

In practice, there are often no clear objectives for many illnesses. Thus, it is not feasible to use the aforementioned methodologies to develop medications for these conditions. Instead of focussing on particular targets, Zhu *et al*.'s deep learning-based effectiveness prediction system (DLEPS) may find potential new drugs by analysing changes in gene expression patterns.75 A convolutional neural network (CNN) was trained to detect changes in gene expression by first encoding molecules using SMILES. We then used a strategy similar to gene set enrichment analysis to rank the chemicals according to their potential anti-disease effectiveness based on gene signatures unique to each illness. When it comes to finding new medications for complicated disorders, DLEPS offers fresh ideas.

Drug-target binding affinity prediction

The majority of the time, the binding affinity between a medication and its target is ignored when DTI prediction is seen as a binary classification problem. A drug's binding affinity provides important insight into the kind and degree of interactions between the medication and its target. It is possible to experimentally estimate binding affinity by measuring dissociation and inhibition constants, but these processes are very expensive and time-consuming. Consequently, it is critical to create computational approaches for estimating binding affinity.

The first deep learning model for predicting the binding affinity of medicines to their targets was proposed by Öztürk *et al*. in 2018, and it was named DeepDTA. As input to CNN, DeepDTA used SMILES to encode the medication and amino acid letters to encode the target. On the right-hand side of the bottom right corner lies the DeepDTA framework. The findings showed that when it came to drug-target binding affinity prediction, DeepDTA reduced both KronRLS and SimBoost. Following DeepDTA's lead, a number of other deep learning-based models-including WideDTA and DeepAffinity-have been developed and are now valuable resources for the pharmaceutical industry.

The effects of medication combinations might be either synergistic or antagonistic. While the latter decreases the efficacy of medications, the former can overcome both primary and secondary drug resistance and is beneficial in treating cancer, AIDS, and bacterial infections. The amount of conceivable medication combinations is staggering, given the ever-increasing number of pharmaceuticals. As a result, studying the effects of medication combinations experimentally is an expensive and time-consuming ordeal. Artificial intelligence (AI) advancements have made it feasible to more efficiently and cheaply explore potential medication combinations.

A Bayesian network model for investigating and evaluating medication combinations was suggested by Li *et al*. in 2015. Predicting compound synergism from chemical-genetic interactions was made possible by a random forest-based model created by Wildenhain *et al*. in the same year. To forecast the synergy of anticancer medications, Preuer *et al*. recently presented DeepSynergy, a model based on deep learning. Drug chemical information and illness genetic information were the inputs of DeepSynergy, which passed them on to the output unit via the network. Using a publicly accessible synergy dataset, researchers found that Deep Synergy was the best at predicting when drugs will work together.

AI in nanomedicine design

One clinical use of nanotechnology is the creation of nanomedicines, which make use of materials with a nanometric size. The materials used to create nanomedicines are on the nanometer scale, which allows them to interact with biological targets despite their size. The United States Food and Drug Administration has previously authorized many nanomedicines, and they have shown improved efficacy in treating cancer and HIV-1 infection. Nevertheless, nanomedicines were not widely used due to a lack of quantitative and qualitative knowledge of the characteristics of nanomaterials and how they interact with living organisms.

Nanotechnology and AI work together to solve this problem in a new way. To optimised the composition of nanomedicine, for instance, Li *et al*. suggested an ANN. In order to forecast the extrusion temperature, filament mechanical characteristics, and dissolution time of nanomaterials, Muñiz Castro *et al*. created a 3D printing nanomaterial formulation process. The absorption of nanomedicines by cells also impacts their efficacy. Scientists will benefit greatly from a cellular uptake prediction model when trying to foretell how successful nanomedicine will be. Alafeef *et al*. built a system to forecast which cell types would internalize nanoparticles

using an ANN. A recent thorough analysis summed up other AI applications to nanomedicine design and related concepts.

AI in oligonucleotide design

A new class of medications called oligonucleotide therapies, which are made up of short strands of DNA or RNA, has emerged alongside pharmaceuticals derived from natural materials. The major oligonucleotide therapeutics systems that allow for the precise therapy of different disorders are antisense oligonucleotides (ASO), small interfering RNA (siRNA), and CRISPR-Cas (clustered regularly inter-spaced short palindromic repeats). Researchers have also turned to AI techniques for assistance in identifying and constructing oligonucleotide-based medications due to the high expense of experimentally designing these oligonucleotides. To find efficient exon skipping ASOs, for instance, Chiba *et al*. presented eSkip-Finder, a technique based on machine learning. To forecast the effectiveness of sirnas, Dar *et al*. created SMEpred.

Conclusion

Researchers, pharmaceutical companies, and regulatory agencies are showing a lot of interest in artificial intelligence drug discovery because of the field's potential to change medicine development processes. The field of drug discovery and development has benefited greatly from the latest advancements in artificial intelligence (AI) models and machine learning (ML/DL) approaches. Additional encouraging developments in the field of drug discovery and development include the Chat Generative Pre-Trained Transformer (ChatGPT), which offers approaches to target identification, drug design, and pharmacodynamic optimization of candidate medications. The accessibility of high-quality data, data curation, and data quantity are three of the many obstacles that AI systems must overcome. It is recommended to use oversampling and under sampling strategies to balance dataset samples, since data quality is essential for AI technology implementations. The lack of interpretability in many models built using AI approaches also makes it hard for experimental scientists to have faith in the predictive outcomes produced by these methods. Approaches including textual explanation, visual explanation, and attention mechanism explanation are proposed as post hoc explanation methods to tackle this problem. Another difficulty in the drug development process is making the suggested models easily accessible. There are a lot of models built on top of AI techniques, but they don't have open-source scripts or web servers. To address these concerns and increase the future value of AI approaches, open-source tools or packages are essential. It is anticipated that AI approaches would bring revolutionary improvements to the area of drug research and development, and despite these hurdles, AI techniques have already been integrated into the industry.

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