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AI-Based Drug Discovery – Revolutionizing Pharmaceutical Research

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Abstract

The traditional drug discovery process is often costly, time-consuming, and prone to high failure rates. The advent of Artificial Intelligence (AI) has revolutionized this field by significantly enhancing efficiency, reducing costs, and improving success rates. AI-driven approaches, including machine learning (ML), deep learning (DL), and natural language processing (NLP), have transformed key areas, such as drug target identification, molecular screening, lead optimization, and clinical trial design. AI models can analyze large-scale biological and chemical data, predict molecular interactions, and optimize drug development pipelines. Applications, like AI-driven virtual screening, AI-enabled gene editing, and predictive toxicology, have demonstrated promising results in accelerating the discovery of novel therapeutics. Additionally, AI technologies, such as Alpha Fold, IBM Watson, and DeepChem are proving instrumental in structure-based drug design and biomarker discovery. However, challenges, such as data quality, ethical considerations, regulatory hurdles, and model interpretability remain key obstacles in AI-driven drug discovery. This review explores the latest advancements in AI-based pharmaceutical research, the impact of AI on various stages of drug development, and potential future directions in this rapidly evolving domain.

Keywords: Artificial intelligence, drug discovery, investigational new drug, investigational new drug, AI-based disease identification

INTRODUCTION

Drug discovery is a systematic scientific process that aims to identify, design, and develop novel therapeutic agents to cure, ameliorate, or prevent diseases and medical conditions. Drug discovery is often called a pipeline, which suggests a unidirectional transition from hit/lead to candidate and marketed drug, supported by basic and clinical research [1–96]. The process is, in fact, iterative in nature, multifaceted, and complex. For example, small-molecule drug discovery requires:

- Basic science research and target identification.
- Target pharmacology and biomarker development.
- Lead identification.
- Lead optimization, candidate selection, investigational new drug (IND)-enabling studies and scale-up for manufacturing.
- Clinical research and development.
- Regulatory review.
- Post marketing.
- Medical practice deployment [2, 97].

Two drug discovery, development and deployment maps (4DMs) that depict key steps in the drug development life cycle, one for small molecules and one for biologics, illustrate the interdependent-denies and complexities of this

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process and are available for download at the National Center for Advancing Translational Sciences (NCATS) website (https://ncats.nih.gov/translation/maps). Drug discovery scientists use various techniques and methodologies, such as computational modeling, medicinal chemistry, high-throughput screening (HTS), and biological assays, to identify promising compounds and evaluate their safety, efficacy, and pharmacokinetics. As therapeutic modalities continue to evolve [3], drug discovery process is adapted by in-corpora ting novel data science, informatics, and artificial intelligence (AI) methodologies, among other technologies, to improve efficiency and reduce costs and animal experiments, thus accelerating the development of novel, effective treatments. The impact of big data and AI in drug discovery, the subject of a 2020 review in this journal [4], continues to attract significant interest: Investors [5, 6], industrial and academic scientists and legislators are discussing the impact of artificial intelligence for drug discovery (AI4DD) [7–11]. As of July 31, 2023, "artificial intelligence in drug discovery" is in the title of 65 publications since 2019, according to Google Scholar (https://bit.ly/3FWk3dH).

INTRODUCTION TO AI AND ITS POTENTIAL FOR USE IN DRUG DISCOVERY

In recent years, there has been a lot of interest in medicinal chemistry's application of artificial intelligence (AI) as a potential way to transform the pharmaceutical sector [12]. The process of finding and creating new drugs, or drug discovery, is a difficult and drawn-out undertaking that has historically relied on time-consuming methods like high-throughput screening and trial-and-error testing. However, by making it possible to analyze vast volumes of data more accurately and efficiently, artificial intelligence (AI) techniques, like machine learning (ML) and natural language processing, have the potential to speed up and enhance this process [13]. The authors have recently reported the successful application of deep learning (DL) to accurately predict the efficacy of medicinal molecules. The toxicity of potential medications has also been predicted by AI-based techniques [14, 15]. These and other studies have demonstrated AI's potential to increase the efficacy and efficiency of drug discovery procedures. But there are drawbacks and restrictions to using AI to create novel bioactive chemicals. To completely comprehend the benefits and limitations of AI in this field, more research is required, and ethical considerations must be considered [16]. Notwithstanding these obstacles, it is anticipated that AI will play a major role in the creation of novel drugs and treatments during the coming years.

TRADITIONAL DRUG DISCOVERY PROCESS

AI in Drug Target Identification

It takes more than ten years and USD 2 billion to create a new drug, and the process is risky, costly, and time-consuming [17]. By 2022, only about 500 viable drug targets had been identified, representing a very small percentage of the anticipated druggable targets in humans [18, 19]. One of the most crucial steps in identifying a disease's biological etiology and developing efficient treatments is target identification [20]. It is the process of selecting appropriate biological molecules or cellular pathways that can be altered by drugs to achieve therapeutic benefits. The availability of biomedical data has increased in recent years, ranging from basic research into the causes of disease to clinical studies. However, this large amount of information poses challenges for data analysis in terms of scalability, data integration, data quality, noise, computational complexity, interpretability, and validation. AI can manage and analyze such complex networks of biological data. Recently, a promising method for target identification has been developed that combines multi-omics data with AI algorithms [21].

Puna et al. prioritized treatable genes and identified prospective therapeutic targets in amyotrophic lateral sclerosis (ALS) by combining different bioinformatics and DL-based models trained using disease-specific text and multi-omics data. This resulted in 18 potential therapeutic targets for ALS. PandaOmics evaluates targets by considering their correlations with certain diseases, as well as data on druggability, developmental stage, and tissue specificity, using more than 20 AI and bioinformatics models. Using advanced DL models and AI techniques, PandaOmics could predict the target genes associated with a specific disease by combining omics AI scores, text-based AI scores, finance scores, and key opinion leaders (KOL) ratings [22]. Eight unreported sites whose removal significantly reduces ocular neurodegeneration were found when suggested AI therapeutic targets for ALS were validated in

a drosophila model that mimics ALS. Additionally, Zhang et al. verified the neurotoxic effects of KANK1 mutations reproduced by CRISPR-Cas9 in human neurons and created an ML-based method to identify KANK1 as a novel ALS-related gene in the same therapeutic area [23]. Zeng et al. created Deep DT net to help with the in-silico identification of molecular targets for medications that are already approved. It is predicated on phenotypic, cellular, genomic, and fifteen distinct kinds of chemical networks. One of the newly developed medications that targets human ROR-γt showed therapeutic efficacy in a mouse model of multiple sclerosis [24]. AI has drawn a lot of attention, and the pharmaceutical business has seen impressive outcomes from ML-based algorithms, particularly AI methodologies [25].

Drug Design and Optimization

The aim of drug design is to obtain small molecules that could meet various criteria, including efficacy for pharmacological purposes, an appropriate safety profile, appropriate chemical and biological properties, and sufficient innovation to secure intellectual property rights for commercial success, etc. [26]. The computational tools have been crucial to drug discovery and have completely changed the way drugs are designed. There are still several problems associated with traditional computational techniques, including input time, computational cost, and reliability [27, 28]. AI could overcome all the obstacles associated with computational drug development, thereby increasing the usefulness of computational techniques in drug development.

AI-Based Disease Identification

AI has demonstrated significant promise in the detection of infectious diseases. Artificial intelligence (AI) can swiftly identify infectious disease epidemics and give early warning systems by evaluating vast volumes of data from several sources, including news reporting, social media, and electronic health records (EHRs). By identifying high-risk communities and monitoring the movements of affected individuals, AI can also help predict the spread of illnesses. AI has the potential to greatly enhance our ability to detect and treat infectious diseases because of its ability to handle vast volumes of data quickly and accurately.AI has made incredible strides in disease diagnosis in recent years, completely changing the way healthcare is provided. Medical practitioners are now able to create extremely precise and trustworthy diagnostic models for a variety of ailments because to AI technologies like ML and DL. The application of AI in disease diagnosis has improved patient outcomes by enabling early detection, accurate diagnosis, and customized treatment options. AI-assisted diagnosis of infectious and non-communicable diseases has advanced significantly in recent years. The diagnosis of infectious diseases has been improved because of AI techniques [29]. The clinical decision support system (CDSS) called "Sepsis Watch" is an excellent example of how to identify sepsis early [30, 98]. This serious illness, which frequently arises from infections in the lungs, urinary system, skin, or gastrointestinal tract, happens when an infection in the body sets off a series of events that can lead to a life-threatening medical emergency [31]. To detect sepsis, Sepsis Watch employs a novel machine learning technique that blends recurrent neural networks (RNNs) with multitask Gaussian processes (MGPs) [31]. For every dynamic variable, the system's MGP component learns the distributions of continuous functions. The RNN, a type of DL that is very good at processing time-series data and crucial for combining both static and dynamic aspects of hospital patient encounters, receives dynamic elements from the MGP hourly, which are then coupled with static features and fed into the system [31].

AI-Enabled Virtual Screening in Drug Discovery

Possibilities and difficulties to find compounds with the desired cellular or biochemical properties, many compounds are often computationally screened in the first step of drug discovery. New techniques are continuously being developed to improve this process's speed, effectiveness, and cost-effectiveness. In a biochemical experiment, primary "hit" chemicals are identified by a positive response during the initial screening phase. Further screening is then carried out to determine whether the hit compounds' physicochemical and pharmacological characteristics are appropriate for creating medication. They are classified as "leads" if they pass these criteria. Before moving on to clinical testing, these leads undergo chemical refinement and biological screening in later stages. Hopefully, a lead will eventually be

approved as a medication, which could take 12 to 15 years after testing starts [32]. Drug development is still a costly and time-consuming procedure, even with major improvements in medicinal chemistry and drug discovery technology. To find hit compounds that may be optimized to lead compounds with desired attributes including higher potency, solubility, and reduced toxicity and off-target effects, thousands of compounds are subjected to in vitro experiments as part of the current standard procedure, which comprises HTS [33].

AI AND GENE EDITING TECHNOLOGIES FOR DEVELOPING GENE THERAPIES

When trying to extract physiologically or therapeutically relevant information from large genotype and phenotype databases, data scientists encounter both opportunities and obstacles due to the increasing amount of genomic and clinical data. Over the past 20 years, data science methods and AI-based technologies have been successfully applied in genomics. The clinical notes, discharge summaries, radiography, and pathology reports that comprise approximately 80% of the unstructured data in EHRs contain a substantial amount of phenotypic information [34]. This information can be extracted from free text using clinical NLP techniques, like cTAKES, which can parse semantic relationships and extract structured concepts. Using NLP approaches in conjunction with both structured and unstructured data has greatly increased phenotyping accuracy. NLP can be added to structured data to improve sensitivity while maintaining a high positive predictive value for several diseases, including inflammatory bowel disease and multiple sclerosis, according to Liao et al.'s examination of the data [35].

The Role of AI in Rare Disease Research

Nearly 3.5 to 5.9% of the world population, people is suffering from rare diseases (RDs), which is a serious health concern [36]. Because of the intricacy of the symptoms and the rarity of the illnesses, diagnosing RDs can be difficult even if they are common. Significant delays in treatment and management may result from a diagnosis that is delayed by up to seven years [37]. New methods are, therefore, required to improve RD diagnosis and treatment. AI based on NB, RF, XG Boost, CNN, AE (autoencoder), RNN, GAN (generative adversarial network), etc. has the potential to revolutionize rare disease detection and treatment [38–40]. To identify tubers in certain MRI (magnetic resonance imaging) images for the diagnosis of tuberous sclerosis complex (TSC), Fernández and colleagues created a deep DL-based method [38–40]. This model shows good performance (accuracy 95%) in the detection of a rare neurological illness by using a special InceptionV3 CNN architecture to determine whether tubers are present in an MRI image. Founta developed a classifier based on XG Boost and RF to diagnose ALS and its distinct subtypes by introducing a semi-automated preprocessing gene selection mechanism to discover causal amyotrophic lateral sclerosis (ALS) genes [39]. The classification accuracy of sporadic ALS motor neuron samples using this methodology was 88.89%. Furthermore, AI-based PET shows promise as a diagnostic and early detection tool for RDs [41].

AI in Clinical Trial Design

Clinical trials, which take six to seven years and a significant financial commitment, are intended to determine the safety and effectiveness of a drug product in people for a specific medical condition. Nevertheless, the industry suffers a significant loss because only one out of ten compounds that undergo these trials are successfully cleared [42]. Poor infrastructure outdated technical requirements, and improper patient selection can all lead to these failures. However, by using AI, these problems can be minimized thanks to the abundance of digital medical data that is currently available [43]. A third of the clinical trials time is spent enrolling in subjects. Finding the right patients is crucial to the success of a clinical study, as failures account for 86% of cases [44].

By employing patient-specific genome–exposome profile analysis, AI can help choose only a certain diseased population for recruitment in Phase II and III clinical trials. This can aid in the early prediction of the possible therapeutic targets in the patients chosen [43–45]. The early prediction of lead molecules that would pass clinical trials while considering the chosen patient population is aided by preclinical

molecule discovery and the prediction of lead compounds prior to the commencement of clinical trials using other facets of AI, such as predictive machine learning and other reasoning techniques [44].

AI In Drug Safety: The Road to Clinical Trials

To guarantee patient safety before first-in-human studies, preclinical safety evaluation is used both in vitro and in vivo testing. From simple single-end point screening to more sophisticated in vitro model systems, such as microphysiology or organ-on-chip models, in vitro toxicology testing is intended to identify toxicities early on that could significantly affect the course of a drug discovery program. These are used either prior to or concurrently with in vivo research. Improvements in this area include the integration of various, more intricate data formats (such as gene expression and cell painting) and the expanded use of imaging for a range of data processing uses. The use of deep learning to identify skin toxicity from an in vitro 3D human skin model is one such instance [45].

KEY AI TECHNOLOGIES USED IN DRUG DISCOVERY

Artificial Intelligence

The computational understanding of intelligence and the creation of creatures that may exhibit these behaviors are the focus of artificial intelligence [46]. These machines and entities are also capable of doing tasks that require human intelligence. The procedure entails collecting information, formulating guidelines for using it, drawing broad or specific conclusions, and finally self-correcting [47]. The main advantage of an AI-based approach is that, even in situations where the underlying mechanism is not under full control, it can build a model by learning from examples. AI is used in healthcare to diagnose and cure a variety of illnesses. Tempus for cancer treatment, IBM Watson for oncology, Path AI for pathology diagnosis, and Insilico Medicine for drug discovery are a few examples [48]. In recent years, the pharmaceutical industry has seen a massive increase in the digitization of data. However, gathering, assessing, and using this knowledge to complex clinical concerns has become increasingly challenging with the introduction of digitalization [46]. Because AI can process enormous amounts of data automatically, this promotes its adoption. As a result, artificial intelligence (AI) includes several state-of-the-art tools and networks that can mimic human intelligence [49, 50].

Machine Learning

Machine learning (ML) is the process of teaching computers to interpret data and draw conclusions from examples and patterns. Unsupervised learning, reinforcement learning, or supervised learning could be the case here. [51, 52]. ML may be used to create prediction models from any data. The dataset needs to be cleaned, outliers removed, and missing values imputed before a model can be built. Important processes include feature extraction, data selection, model construction, evaluation, and key attribute and algorithm selection [53, 54]. With machine learning, important phases include data selection, feature extraction, choosing important attributes and algorithms, developing a model, and evaluating the model [54, 55].

Supervised Machine Learning

Supervised machine learning (ML) uses labeled datasets to train algorithms for data classification or precise result prediction. The model updates the weights using a reinforcement learning (RL) technique once input is given to make sure the model fits well. Supervised learning is used by many organizations and sectors to handle supervised machine learning (ML). The model updates the weights using a reinforcement learning (RL) technique once input is given to make sure the model fits correctly. Supervised learning is used by many organizations and businesses to solve a variety of real-world problems. Regression and classification are the two categories of supervised learning [56].

Unsupervised Machine Learning

Unsupervised learning is used when there is an input variable but no output variable. Its main goal is to understand data distribution to get better. It is further separated into clustering and association [56].

Reinforcement Learning

RL is a fascinating subfield of machine learning that has drawn a lot of attention from both academic and business communities. RL is a continuous learning technique that maintains autonomy, as opposed to supervised and unsupervised learning. RL is used in robotics, gaming, and trading because of its quick response to changing conditions (Table 1) [57].

Table 1. AI-based drug discovery-revolutionizing pharmaceutical research.

List of AI-based Software for Drug Discovery [61, 62]			
Tools	***Details***	***Website URL***	***Reference***
Deep Neural NetQSAR	Python-based system driven by computational tools that aid detection of the molecular activity of compounds	https://github.com/Merck/Deep NeuralNet-QSAR	[63]
Deep Chem	MLP model that uses a python-based AI system to find a suitable candidate in drug discovery	https://github.com/deepchem/deepchem	[64]
ORGANIC	A molecular generation tool that helps to create molecules with desired properties. https://github.com/aspuru-guzik-group/ORGANIC	https://github.com/aspuru-guzikgroup/ORGANIC	[65]
Potential Net	Uses NN stop redict binding affinity of ligands https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	[62]
Hit Dexter	ML technique to predict molecules that might respond to biochemical assays. http://hitdexter2.zbh.uni-hamburg.de	http://hitdexter2.zbh.uni-hamburg.de	[61]
Delta Vina	A scoring function for rescoring drug–ligand binding affinity. https://github.com/chengwang88/deltavina	https://github.com/chengwang88/deltavina	[61]
Neura graph fingerprint	Helps to predict properties of novel molecules. https://github.com/HIPS/neural fingerprint	https://github.com/HIPS/neural fingerprint	[61]
DeepTox	Software that predicts the toxicity of total of 12000 drugs. www.bioinf.jku.at/ research/DeepTox	www.bioinf.jku.at/research/Deep Tox	[66]
Alpha Fold	Predicts 3 D structures of proteins. https://deepmind.com/blog/alphafold	https://deepmind.com/blog/alpha fold	[61]
Chemputer	Helps to report procedure for chemical synthesis in standardized format. https://zenodo.org/record/1481731	https://zenodo.org/record/ 1481731	[61]

Deep Learning DL

Deep learning (DL) is a subset of machine learning (ML) in which the system learns on its own from unlabeled and unstructured data. In the late 20th century, Igor Aizenberg et al. [58] referred to an artificial neural network (ANN) as "deep learning". In DL, ANNs with several processing layers are employed [52]. When faced with challenging tasks involving vast quantities of high-dimensional data, DL performs exceptionally well. However, it requires more calculations than traditional machine learning, and because many of the processing layers are hidden from the user, it is commonly referred to as an "AI black box." Thus, there are more risks and challenges in comprehending the concept. Large Language Models (LLMs) are DL models that generate language that is like that of humans by being trained on large datasets. LLMs comprise chatbots, like Chat GPT and GPT-4, that are built on pre-trained generative transformer (GPT) architecture [59]. However, it requires more calculations than traditional machine learning, and because many of the processing layers are hidden from the user, it is commonly referred to as an "AI black box." Thus, there are more risks and challenges in comprehending the concept. Large Language Models (LLMs) are DL models that generate language that is like that of humans by being trained on large datasets. Chat bots, like Chat GPT and GPT-4, which are based on pre-trained generative transformer (GPT) architecture, are a part of LLMs [58]. It does more

calculations than traditional machine learning and is frequently referred to as a "black box" of AI because many of its processing layers are hidden from the user. Hence there are additional difficulties and dangers in understanding the model. Large Language Models (LLMs) are DL models that are trained on big datasets to produce human-like language.

AI-Based Tools in Drug Discovery

The advent of AI technologies is set to transform the landscape of drug discovery by enabling researchers to efficiently navigate vast datasets, innovate molecular structures, and predict the efficacy of potential drug candidates [60].

AlphaFold

Alpha Fold, a ground-breaking AI tool based on DNNs, has advanced significantly in 3D protein structure prediction [67]. AlphaFold has a great success rate in precisely predicting the structure of target proteins by examining the angles of peptide bonds and the distances between neighboring amino acids. AlphaFold has demonstrated its revolutionary skills in protein structure prediction by correctly predicting 25 out of 43 protein structures [60, 61, 68, 71].

IBM Watson

With its extensive natural language processing capabilities and ability to extract logical conclusions from both structured and unstructured input, this AI development milestone was a major accomplishment [68, 72]. Its superiority over two human champions on the game show Jeopardy in 2011 garnered international recognition. This accomplishment was made possible by DeepQA, an advanced natural language processing program created by IBM that allowed Watson to comprehend queries in a remarkable amount of detail and produce precise responses [68–75]. To provide many answers to a given query, DeepQA integrates multiple modules and collects evidence from various databases to support each possible response. During the training phase, these responses are then assessed using a multilayer logistic regression, and the most convincing responses are put to the test to determine which response is the most accurate.

DeepChem

An open-source deep learning platform called DeepChem was created especially to make it easier to apply AI methods to cheminformatics and drug discovery jobs [73]. DeepChem, a Python-based platform, offers an extensive suite of tools for utilizing deep learning in a variety of drug research contexts, ranging from lead optimization and virtual screening to predictive drug property modeling. The Molecule Net dataset, which contains the properties of over 700,000 chemicals and is a useful tool for training and verifying deep learning models in drug discovery, is one of DeepChem's primary features [76]. DeepChem has been used in a wide range of algorithmic research initiatives, such as the creation of one-shot deep learning algorithms for drug discovery and a variety of other applications like protein structure analysis and inhibitor modeling for Alzheimer's disease targets [74–80].

DeepTox

One program that is especially made to forecast the possible toxicity of different medications is called DeepTox. It is a useful tool in the vital process of drug safety evaluation because of its capacity to evaluate many medications at once. DeepTox makes use of deep learning, a type of machine learning that excels at processing intricate, multi-layered data. This enables DeepTox to extract extremely informative chemical characteristics by learning and predicting a variety of possible hazardous effects within a single neural network [69].

Hit Dexter

A machine learning technique called struck Dexter was created to find chemicals that are frequently struck [77]. By including both primary screening and confirmatory dose-response assays, this approach builds on its predecessor. Several machine learning approaches, such as Extremely Randomized Trees

(ETC), Random Forests (RF), AdaBoost, and Bagging Classifiers, were used in the development process [77, 78]. The best results were obtained by the ETC model, whose Matthews Correlation Coefficient (MCC) values ranged from 0.56 to 0.58. With MCC values up to 0.64 and Area Under the Receiver Operating Characteristic Curve (AUROC) values up to 0.96, external validation showed that the best models could categorize promiscuous and no promiscuous substances. The ability of Hit Dexter to forecast promiscuity among approved medications is a major benefit. About 13% of marketed medications were found to be potentially promiscuous by the model, while 6% were categorized as extremely promiscuous. Furthermore, by supporting a wide range of chemical spaces, such as dark chemical matter, aggregators, high-throughput screening (HTS) compounds, drug-like molecules, pan-assay interference compounds (PAINS), and natural goods, the web server exhibits adaptability. Users can access the integrated machine learning models and criteria for identifying frequent hitters and substructures that might be detrimental to drug discovery efforts through Hit Dexter's online accessibility (http://hitdexter2.zbh.uni-hamburg.de) [77, 78].

APPLICATION OF AI IN DRUG DISCOVERY

Drug research is one sector where artificial intelligence (AI) is having a particularly significant impact. AI is revolutionizing many other sectors. AI technologies have the potential to greatly speed up and optimize the drug discovery process, which now takes years and substantial resources. Target identification, drug design, biomarker discovery, clinical trial design, and even post-market surveillance are all phases of drug discovery where artificial intelligence is being used. The main uses of AI in drug discovery are listed below. AI-powered technologies are being utilized to find new therapeutic targets and confirm their applicability to various illnesses. AI models can forecast which genes or proteins are most likely to be implicated in disease processes by examining enormous volumes of biological data, such as transcriptomics, proteomics, and genomics data [79]. Algorithms for machine learning (ML) can examine proteomic and genomic data to find proteins that may be the target of medication. For example, protein-protein interactions – which are essential for comprehending disease mechanisms have been predicted using deep learning models [79]. For instance, by examining vast amounts of patient genomic data, AI methods have been applied in cancer research to find possible targets for precision medicine and immunotherapy [80].

Drug Design and Compound Screening

- AI is transforming drug design by using computational techniques to create new molecules that resemble pharmaceuticals and forecast their characteristics. AI methods, like deep learning, reinforcement learning, and generative models, aid in the creation of novel compounds with minimal toxicity, ideal binding affinities, and drug-like characteristics.
- Reinforcement learning techniques and Generative Adversarial Networks (GANs) can suggest novel chemical compositions that are probably effective against targets. To forecast molecular structures that display the intended pharmacological activity, artificial intelligence systems have been trained [81].
- AI-powered virtual screening techniques can quickly assess enormous chemical libraries to forecast their biological action. Deep neural networks (DNNs), for instance, are used to forecast the interactions of drugs with certain proteins or receptors [82].

Predicting Drug Toxicity and Side Effects

- Early in the drug discovery process, artificial intelligence (AI) is being used to forecast a compound's toxicity, preventing expensive and time-consuming clinical trial failures. To forecast adverse drug reactions (ADRs), machine learning algorithms examine chemical structures, biological interactions, and toxicological data.
- Toxicology prediction models determine possible hazardous effects of substances by using historical data and molecular characteristics. For instance, depending on the molecular structure, deep learning algorithms can forecast cardiac or liver harm [83].

- Tox21 and other AI-powered databases offer substantial datasets that train machine learning models to forecast the toxicity levels and possible adverse effects of novel medication candidates [83].

Biomarker Discovery and Patient Stratification

- AI methods are being used to find disease biomarkers, which can aid in early diagnosis and the development of individualized treatment plans. To stratify patients according to their genetic composition, the course of their disease, and how well they are likely to respond to treatment, biomarkers are essential.
- Clinical, genetic, and imaging data can all be combined by AI algorithms to find biomarkers that predict patient outcomes. For instance, multi-omics data (genomics, proteomics, etc.) have been analyzed using machine learning to find biomarkers for conditions including cancer, Alzheimer's, and cardiovascular disorders [84].
- To create more individualized treatment strategies, patient stratification techniques also employ AI to divide patients into subgroups according to their genetic, molecular, or clinical characteristics [85].

Optimization of Clinical Trials

- By enhancing patient recruitment, trial design, and monitoring, artificial intelligence is revolutionizing clinical trials. By predicting which patients are most likely to respond to a certain treatment, artificial intelligence (AI) techniques can optimize the enrollment process.
- AI-driven algorithms can analyze patient records, genomics, and clinical data to identify eligible patients more efficiently, thereby speeding up recruitment [86].
- Furthermore, by forecasting patient outcomes and recommending the best course of therapy, AI models can improve trial design.
- AI-powered adaptive trial designs increase efficiency and lower costs by enabling real-time monitoring and trial parameter adjustments based on continuous data [82].

Post-Market Surveillance

- AI is essential in tracking a drug's effectiveness in real-world situations after it has been approved. AI is used in post-market monitoring to monitor long-term efficacy, adverse events, and drug interactions in a variety of patient populations.
- Natural language processing (NLP) and machine learning techniques are employed to analyze electronic health records (EHRs), social media, and other sources to detect previously unidentified side effects or complications [86].
- To identify trends in drug safety signals and forecast possible public health hazards, AI models can also examine global pharmacovigilance data [87].

CHALLENGES AND LIMITATIONS OF USING AI IN DRUG DISCOVERY

Notwithstanding the potential advantages of AI in drug discovery, several restrictions and difficulties need to be considered. The availability of appropriate data is one of the main obstacles [88]. Large amounts of data are usually needed for training in AI-based methods [89]. The accuracy and dependability of the results may be impacted by the fact that there is frequently a lack of available data or that the data is inconsistent or of poor quality [90]. Since AI-based methods may give rise to questions regarding prejudice and fairness (see the following section), ethical considerations create another difficulty [91, 92]. For instance, predictions made by an ML system may be unfair or erroneous if the data used to train the algorithm is biased or unrepresentative [93]. One crucial issue that needs to be addressed is making sure AI is used fairly and ethically while developing novel medicinal molecules [94]. The challenges that AI faces in the field of chemical medicine can be addressed in several ways. One strategy is data augmentation [95].

Ongoing Challenges in Adopting AI: Leads on Ways to Overcome

Since these data are utilized for the system's subsequent training, the availability of a significant volume of data is essential to the success of AI. A business may have to pay more to get data from

several database providers, and for accurate prediction, the data must be high-quality and dependable. The lack of qualified staff to run AI-based platforms, small businesses' tight budgets, concerns about replacing humans and losing jobs, doubts about the data produced by AI, and the "black box" phenomenon – the process by which the AI platform draws its conclusions – are additional obstacles to the full-fledged adoption of AI in the pharmaceutical sector.

FUTURE PERSPECTIVE

AI can completely transform pharmaceutical research by accelerating the discovery and creation of new medications. Both ML and DL algorithms are widely used in the pharmaceutical industry. However, there have been a lot of discussions about machine learning techniques, particularly in the areas of image analysis and omics data. It is anticipated that the application of AI to rapidly predict biological targets and innovative leads will significantly reduce the time required for drug discovery and the probability of failures at later stages.

Drug reuse and repurposing may be significantly impacted by the discovery of new therapeutic indications. By accelerating the process of discovering and creating new medications, DL AI has the potential to completely transform the pharmaceutical sector in the coming ten years. Both ML and DL algorithms are widely used in the pharmaceutical industry. However, there have been a lot of discussions about machine learning techniques, particularly in the areas of image analysis and omics data. It is anticipated that the application of AI to rapidly predict biological targets and innovative leads will significantly reduce the time required for drug discovery and the probability of failures at later stages. Drug reuse and repurposing may be significantly impacted by the discovery of new therapeutic indications. DL has advanced significantly over the past ten years in several AI research areas, including natural language processing and audio and image recognition. It has been demonstrated that applying edge detection, picture categorization, and filters improves data analysis results. The biological techniques used in the initial stages of drug development require further research in the field of machine learning in addition to quantum machine learning. For instance, a constrained Boltzmann machine's training time can be shortened using quantum computers. Recently, DL techniques have been used to predict the locations of ligand binding. However, every DL technique now in use is based on the widely used convolutional/recurrent network design [96, 97].

CONCLUSIONS

Artificial Intelligence (AI) is revolutionizing the field of drug discovery by accelerating the identification of potential drug candidates, optimizing lead compounds, and improving clinical trial design. AI-driven approaches, such as machine learning, deep learning, and natural language processing have significantly enhanced efficiency, reduced development costs, and minimized failure rates in drug development. The integration of AI into drug discovery has enabled rapid screening of compounds, accurate prediction of molecular interactions, and precise identification of drug gable targets. Additionally, AI has shown remarkable potential in rare disease research, drug repurpose, and personalized medicine. Despite these advancements, several challenges remain, including data quality, regulatory hurdles, ethical considerations, and the interpretability of AI models. The adoption of standardized AI frameworks, improved validation techniques, and enhanced collaboration between AI experts and pharmaceutical scientists will be crucial for overcoming these challenges. Looking ahead, the future of AI-driven drug discovery is promising, with emerging technologies, like quantum computing and generative AI, expected to further refine the process. AI has the potential to transform pharmaceutical research, leading to faster and more cost-effective drug development, ultimately improving global healthcare outcomes.

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