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Artificial Intelligence in Drug Discovery and Development

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Abstract:
The drug discovery and development process is very lengthy, highly expensive, and extremely complex in nature. Considering the time and cost constraints associated with conventional drug discovery, new methods must be found to enhance the declining efficiency of traditional approaches. Artificial intelligence (AI) has emerged as a powerful tool that harnesses anthropomorphic knowledge and provides expedited solutions to complex challenges. Advancements in AI and machine learning (ML) techniques have revolutionized their applications to drug discovery and development. This review illuminates the profound influence of AI on diverse aspects of drug discovery, encompassing drug-target identification, molecular properties, compound analysis, drug development, quality assurance, and drug toxicity assessment. ML algorithms play an important role in testing systems and can predict important aspects such as the pharmacokinetics and toxicity of drug candidates. This review not only strengthens the theoretical foundation and development of this technology, but also explores the myriad challenges and promising prospects of AI in drug discovery and development. The combination of AI and drug discovery offers a promising strategy to overcome the challenges and complexities of the pharmaceutical industry.

Keywords: artificial intelligence; machine learning; deep learning; drug discovery.

INTRODUCTION
Drug discovery has existed for almost as old as human history, it started with serendipitous discovery and gradually evolved into a process that was strongly based on scientific evidence and involved multidisciplinary studies. A historical perspective on drug discovery offers a deeper understanding of the drug discovery process. It is important in sharpening the vision of the present as well as the future of drug discovery research. In the past 20 years, reviews on the transformation of drug discovery have been scarce. Umashanka & Gurunathan (2015) provided a brief view of the transition from traditional drug discovery to modern drug discovery and particularly emphasised the protocol involved in drug development, Drews (2000) reviewed the impacts of molecular biology on drug discovery development while Gershell and Atkins (2003) focused on the pivotal technologies in the drug discovery process. On the other hand, Villoutreix (2021) presented challenges of drug discovery after the COVID 19 pandemic (Drews, 2000; Gershell & Atkins, 2003; Umashankar & Gurunathan, 2015; Villoutreix, 2021). Most papers reviewed drug discovery in specific areas, subject matters, methods, or applications including natural products drug discovery, peptide drug discovery, the role of nanobiotechnology in drug discovery, computational approaches in drug discoveryand antiviral and antibacterial drug discovery, etc (Campbell., 2017; George, 2022; Henninot, 2018; Katz & Baltz, 2016; Moffat, 2014; Ong & Gasser, 2022; Pettersson & Crews, 2019; Totura & Bavari, 2019; Tse., 2019). Review on the development of drug discovery research from the past to the present is scarce, and the relevant information can mostly be found in books. The books authored by Gerald (2013), Sinha & Vohora (2018), and Hill & Richards (2021) are some of the examples that discussed general drug discovery and development (Gerald, 2013; Hill & Richards, 2021; Sinha & Vohora, 2018). In this paper, we reviewed drug discovery from historical perspectives and highlighted some achievements in the past.[1-4]

Drug discovery in ancient time
Some studies have reported Paleolithic humans knew about using bitter plants with poison or psychotropic plants for self-medication (Hardy, 2021). Around 10,000 years ago, the human race settled from nomad life and grow their plants for food, setting off the agricultural evolution that brought civilization as well as plagues of infectious diseases (Abbo., 2022; Hill & Richards, 2021). In the ancient past, there was no system of medicine, the primary source of medicine for the treatment of diseases was plants which were mostly discovered by chance. Some of the “drugs” discovered were without medicinal value such as alcohol and tea, while some others are harmful and addictive such as cannabis and opium (Gerald, 2013). The functions of plants as medicines were transmitted verbally or engraved on caves and the practices were greatly affected by the cultures and religions (Pina, 2010; Poduri, 2021).

1.Drug discovery from the 18th century to 19th century
Highlights of drug discovery research from the 18th century to 19th century

- **Drug discovery in the 18th century**

In the 18th century, the practices of clinical trials and preventive medicine were started when James Lind reported his study on the prevention of scurvy with his established first controlled clinical study in 1753 which founded the concept of scientific testing on drug efficacy (Gerald, 2013; Hill &

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Richards, 2021). In 1796, the first vaccine was born when an English physician Edward Jenner used cowpox to immunize people for the prevention of smallpox which eventually led to the eradication of smallpox diseases in 1979 (Gerald, 2013). In the same year, homeopathic medicine was founded by Samuel Hahnemann (Gerald, 2013).

2. **Drug discovery in the 19th century**

In the 19th century, the advancement of chemistry allowed the extraction and isolation of active substances from herbal plants bringing drug discovery to small molecule drug discovery. In the early 1800s, important active substances such as alkaloids, morphine, quinine, and atropine were first extracted and isolated from the plants (Gerald, 2013). Morphine is still the most effective painkiller for severe pain today. In the interim, the advance of synthetic chemistry led to the production of Aspirin, the blockbuster drug derived from salicylic acid extracted from the plant and is still one of the most widely used drugs in the world. Aspirin was marketed as an analgesic in 1899 and was effective in relieving pain and anti-inflammation. In 1982, owing to the antiplatelet effect of aspirin, it was repurposed for use in cardiovascular disease and more functions of aspirin are still under study (Jourdan et al., 2020; Gerald, 2013). Progress in biomedicine was also observed in the 19th century.

3. Drug discovery since the 20thcentury

Highlights of drug discovery research since the 20th century

Drugs that did not originate from plants started to be produced. In the early 20th century, heparin isolated from dog's livers and insulin from dog's pancreas were used to treat blood clots and severe diabetes respectively. Antibiotic drugs such as penicillin, ciclosporin, and tacrolimus were isolated from the fungus while streptomycin and tetracyclines were isolated from soil bacteria (Clardy, 2009). Penicillin is the first antibiotic drug discovered by Alexander Fleming in 1928 has saved numerous lives. Later, the successful elucidation of penicillin structure subsequently produced many other structure-related antibiotics such as ampicillin. Penicillin remains one of the most commonly used antibiotics today (Gerald, 2013; 2009; Yip & Gerriets, 2022). In the 1880s, acetanilide was discovered to be able to diminish fever, however, it was also found to cause hematotoxicity.

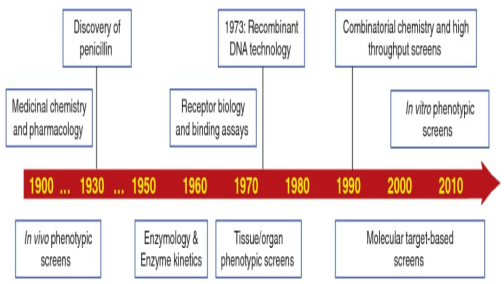

Fig:1 Drug Discovey in Ancient Times

4. Development of recombinant DNA

Discoveries of restriction enzymes started in the 1950s and the first experiment was conducted in 1971 (Felice, 2019). This set off the development of recombinant DNA and transformed the chemistry-based drug discovery industry (Bose & Bose, 2022; Gershell & Atkins, 2003). This enabled the production of the first peptide based drug, Humulin or human insulin in 1982. Since then, not only peptide-based drugs but biological drugs also have been produced such as trastuzumab (Herceptin), which is a monoclonal antibody made in 1998 (Gershell & Atkins, 2003; Wang, 2022).

- **Molecular biology directed drug discovery**

One of the biggest contributions to molecular biology and drug discovery research is the initiation of the Human Genome Project (HGP). The idea of HGP was conceived in 1984, then the project was commenced in 1990 and took 15 years to finish and eventually launched a post-genomic era (Hood & Rowen, 2013; Woollard , 2011; Yan, 2015). The HGP has benefited many sectors more than what scientists had expected of it when initiated the project as it has led drug discovery research to a new paradigm shift. Along the way, it set off the application of "big data" science, fostered the development of omics technologies and the advancement of multi disciplines such as computational and mathematics (Hood & Rowen, 2013; Woollard, 2011).

5. AI in disease identification and clinical diagnosis

Laboratory investigations and clinical examinations are the most common methods used in clinical diagnosis, which is a the fundamental step in providing high-quality treatments. The remarkable ability of AI techniques in Clinical Diagnosis Decision Support (CDDS) has acquired a significant interest in medical research in recent years. The incorporation of AI in clinical workflows provides abundant opportunities to reduce clinical errors, improve treatment outcomes, lower treatment costs, detect diseases at earlier stages, and track treatment progress over time. In this section, we will elaborate on the recent studies that have reported the use of AI technology for clinical disease diagnosis. Furthermore, we will highlight the applications of AI in genome analysis and personalized medicine

6. AI in genome analysis

Around 80% of rare diseases are related to genetic variations. Hence, the importance of diagnoses provided by genome sequencing. The advancements in Next Generation Sequencing (NGS) technology have led to the collection of vast amounts of data and provided rich information about individual genomes. The bottleneck in NGS lies in the analysis and interpretation of large-scale genome data and the identification of variants. This can take days to weeks. AI-based models, such as deep learning models, opened a new chapter of research related to transforming this 'big data' into meaningful new information. AI technology has been applied in many areas of genomic analysis such as gene annotation, genotype-phenotype correlations, consanguinity diseases, mutation studies, cancer diagnosis, biomarker identification, gene function prediction, and variant calling. Another challenge in the analysis of genome sequences is to distinguish benign from disease-causing gene variants for rare genetic disorders. In a collaborative retrospective study between the company Fabric Genomics and Rady Children's Institute, San Diego, researchers built an automated AI algorithm called

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Fabric GEM (where GEM stands for genomics). They used 179 diagnosed pediatric cases, mostly from the Neonatal intensive care unit (NICU) at Rady Children's Institute, and five other clinics across the world.

7. AI in personalized medicine

Traditionally, clinical practice has been based on the concept of 'one therapy fits all'. However, drug molecules may undergo different metabolic activities in different patients. For example, a drug that works well for a group of people may not be as effective, or may have adverse side effects, for others. These differences in drug metabolism are mostly attributed to the differences in the genetic profile of individuals. Thus, a more futuristic approach is a personalized treatment, also known as precision medicine, where patients are treated based on their genetic profile. The aim is to maximize treatment outcomes while minimizing adverse effects per individual. Thus, different therapies and doses are customized per individual (or per group of patients that share similar genome profiles).[5-8]

Overview of Drug Discovery and Development Process

The process of bringing a new pharmaceutical product to market involves a series of carefully regulated and scientifically rigorous steps, typically categorized into drug discovery and drug development phases. Each stage is critical to ensuring that the final drug product is safe, effective, and suitable for human use. However, the traditional drug development pipeline is characterized by significant costs, long timelines, and high failure rates, with estimates suggesting that it may take 10–15 years and over \$2 billion to develop a single successful drug. Understanding these steps provides a framework to appreciate how artificial intelligence (AI) can intervene and improve efficiency at various stages.[9-12]

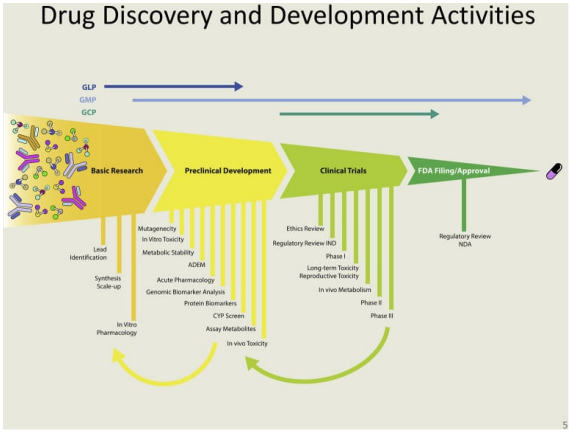

Fig:2 Drug Discovery & Development

Drug Discovery

The drug discovery phase focuses on identifying and validating biological targets and finding chemical compounds that can modulate those targets to produce a desired therapeutic effect. Target Identification and Validation: This initial step involves selecting biological molecules—typically proteins, genes, or RNA—that play a role in a particular disease. Experimental methods like genomics, proteomics, and transcriptomics, along with literature mining, are commonly used. The challenge lies in the complexity of biological systems and the difficulty in predicting which targets will be both efficacious and safe. Hit Identification: Once a target is validated, libraries of chemical compounds are screened using high-throughput screening (HTS) or virtual screening to identify potential "hits" — compounds that interact with the target. This stage generates large volumes of data that require advanced analytics. Lead Optimization: Hits undergo chemical modifications to improve their pharmacodynamic and pharmacokinetic properties. This iterative process involves structure activity relationship (SAR) studies, toxicity assessments, and solubility improvements, among other considerations. In Vitro and In Vivo Studies: Promising compounds are then tested in cell-based and animalmodels to evaluate efficacy, toxicity, metabolism, and bioavailability before progressing to human trials.

- **Role of AI in Drug Discovery**

Drug discovery is the foundation of the pharmaceutical pipeline, involving the identification of new therapeutic compounds that can modulate disease-related targets. Traditionally, this process is time-consuming, expensive, and characterized by high attrition rates. Artificial Intelligence (AI) has emerged as a game-changing technology, enabling more accurate predictions, faster processing, and better decision-making. From identifying novel biological targets to designing drug-like molecules, AI has begun to enhance nearly every step of the discovery process.

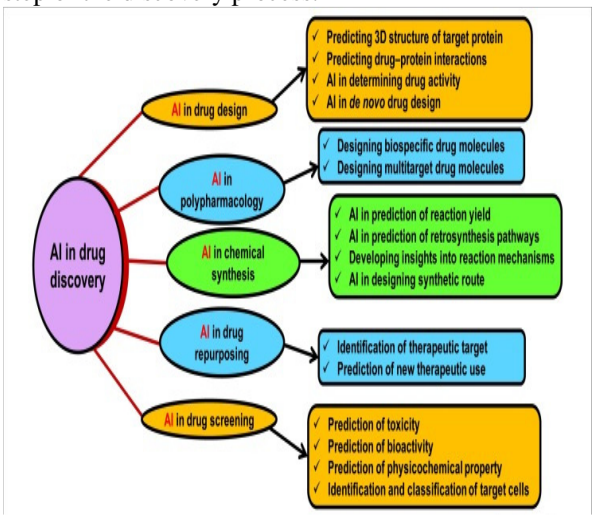

Fig:3 AI in Drug Discovery

4.2 Compound Screening and Hit Identification

High-throughput screening (HTS) has been a standard method for identifying "hits" compounds that exhibit biological activity against a target. AI enhances this stage by: Replacing or supplementing HTS with virtual screening, which reduces the need for physical testing. Using machine learning classifiers (e.g., random forests, support vector machines, neural networks) to predict the bioactivity of thousands of compounds. QSAR (Quantitative Structure–Activity Relationship) modeling to predict how chemical structure affects biological activity.Example: Atomwise uses convolutional neural networks to predict protein-ligand interactions and screen vast chemical libraries in silico

4.3 Lead Optimization

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After hit identification, compounds must be optimized to improve their pharmacokinetic and pharmacodynamic profiles . AI contributes by: Predicting ADMET properties (absorption, distribution, metabolism, excretion, toxicity) with high accuracy. Guiding chemical modifications to improve efficacy, selectivity, and bioavailability. Reinforcement learning and generative models for de novo drug design, creating molecules that meet multiple constraints. Example: Insilico Medicine's AI platform designs novel compounds and ranks them based on multiple desirable properties, reducing the trial-and-error aspect of medicinal chemistry.

2.Drug Development

Once a candidate drug demonstrates adequate preclinical performance, it enters the formal drug development stage, which includes clinical trials and regulatory approval processes. Preclinical Development: This stage includes further safety and efficacy studies, toxicity profiling, pharmacokinetics (absorption, distribution, metabolism, and excretion or ADME), and pharmacodynamics. Data generated here supports the Investigational New Drug (IND) application required to begin human testing Clinical Trials: Clinical development occurs in three main phases: Phase I: Small-scale studies (20–100 healthy volunteers) assess safety, dosage range, and pharmacokinetics. Phase II: Larger studies (100–300 patients) evaluate efficacy and side effects in patients with the target disease. Phase III: Large-scale trials (1,000–3,000 patients) confirm efficacy, monitor adverse reactions, and compare the drug with standard treatments. Regulatory Review and Approval: After successful clinical trials, a New Drug Application (NDA) or Marketing Authorization Application (MAA) is submitted to regulatory agencies (e.g., FDA, EMA). This includes comprehensive data on preclinical, clinical, and manufacturing aspects. Post-Marketing Surveillance (Phase IV): Even after approval, the drug is monitored for long-term safety and effectiveness. Pharmacovigilance plays a crucial role in identifying rare adverse effects and ensuring ongoing patient safety.

2.3 Challenges in the Traditional Pipeline

The traditional drug development process faces several systemic challenges: High attrition rates, particularly in clinical phases Difficulty in translating preclinical findings to human biology Rising R\&D costs with diminishing returns Inefficient patient recruitment and trial design Regulatory hurdles and data overloadThese challenges underscore the urgent need for innovative technologies, such as AI, to enhance efficiency, reduce costs, and improve success rates. In the following sections, we explore how AI technologies are being integrated into each of these stages to optimize drug discovery and development.

Role of AI in Drug Development

While AI has significantly transformed drug discovery, its impact is equally profound in the subsequent stages of drug development. This phase includes preclinical testing, clinical trials, regulatory review, and post-market surveillance. AI contributes to making this process more efficient, predictive, and patient-centric by leveraging real-time data, advanced analytics, and automation. These innovations help reduce development costs, shorten timelines, and improve the overall success rate of drug candidates.[13-17]

AI: networks and tools

AI involves several method domains, such as reasoning, knowledge representation, solution search, and, among them, a fundamental paradigm of machine learning (ML). ML uses algorithms that can recognize patterns within a set of data that has been further classified. A subfield of the ML is deep learning (DL), which engages artificial neural networks (ANNs). These comprise a set of interconnected sophisticated computing elements involving 'perceptons' analogous to human biological neurons, mimicking the transmission of electrical impulses in the human brain. ANNs constitute a set of nodes, each receiving a separate input, ultimately converting them to output, either singly or multi-linked using algorithms to solve problems . ANNs involve various types, including multilayer perceptron (MLP) networks, recurrent neural networks (RNNs), and convolutional neural networks (CNNs), which utilize either supervised or unsupervised training procedures.

The MLP network has applications including pattern recognition, optimization aids, process identification, and controls, are usually trained by supervised training procedures operating in a single direction only, and can be used as universal pattern classifiers . RNNs are networks with a closed-loop, having the capability to memorize and store information, such as Boltzmann constants and Hopfield networks. CNNs are a series of dynamic systems with local connections, characterized by its topology, and have use in image and video processing, biological system modeling, processing complex brain functions, pattern recognition, and sophisticated signal processing. The more complex forms include Kohonen networks, RBF networks, LVQ networks, counter-propagation networks, and ADALINE networks.

Several tools have been developed based on the networks that form the core architecture of AI systems. One such tool developed using AI technology is the International Business Machine (IBM) Watson supercomputer (IBM, New York, USA). It was designed to assist in the analysis of a patient's medical information and its correlation with a vast database, resulting in suggesting treatment strategies for cancer. This system can also be used for the rapid detection of diseases.[18-22]

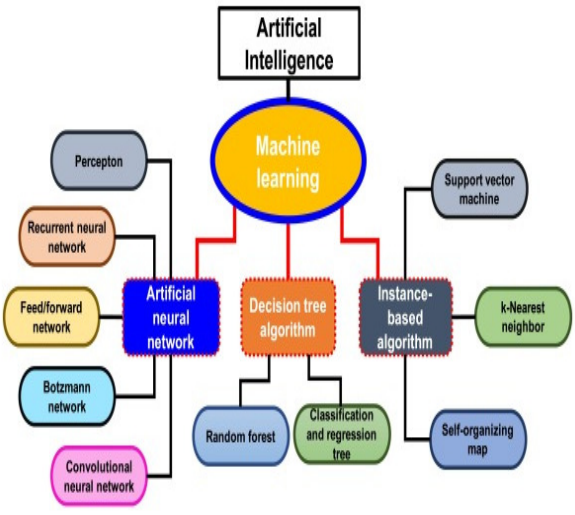

Fig:4 Machine Learning

AI in drug development and clinical trials

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since its inception AI has been readily studied for its ability to enhance the conduction of clinical trials, and certain modifications to the current AI models can make them more compatible with clinical trials.

- **Conventional drug development and clinical trial phases**

Drug development and its associated clinical trials are now faster with more resources as compared to the old-fashioned, time-consuming, and resource-consumptive procedures. The ability to use machine learning models, predictive analytics, and AI-based monitoring tools facilitates pharmaceutical companies accelerating the end-to-end clinical trial design, patient recruitment, and monitoring, resulting in new therapies hitting the markets faster table-1

Clinical trial stage	AI tools/method	Function	Example
Patient recruitment	Predictive analytics, EHR analysis	Identify ideal candidates based on genetic and clinical data	Tempus for cancer trials
Trial design optimization	*In silico* simulation . ML models	Optimize trial structure (*e.g.* dosage duration)	Pfizer AI-optimized trial for vaccines
Real time monitoring	NLP, image recognition	Monitor patient outcomes and adverse reactions in real time	AI powered wearable device

Table:1 AI in clinical trails

Optimizing clinical trial design

These are also the costliest and most time-consuming activities of drug development, taking years and millions of dollars. The new applications of AI provide a solution to both problems. It can optimize the design of a clinical trial, predict patient outcomes, and even conduct virtual trials through *in silico* simulations. ML models driven by AI can analyse huge datasets from previous trials, electronic health records, and genomic data to identify patterns that researchers can use in their research for developing more effective trials.

***In silico* simulations.** AI allows *in silico* or computer-based trials in which algorithms could mimic human trials by using large volumes of biological data, thereby enabling scientists to predict the safety and efficacy of drugs even before real physical trials begin. Pharmaceutical companies could quickly check several clinical scenarios and figure out the most promising candidates through fewer physical trials by saving much time and resources.

Design optimization. The machine-learning algorithms can be used to optimize the parameters of the clinical trials, for example, selecting perfect demographics and determining the right dose and the right time of the clinical trial. AI assists in creating the designs, so that maximum chances of success are there with minimum risk on patients as well as on resources, in addition to modelling based on historical time outcomes. Machine learning models can simulate different clinical trial designs to predict potential outcomes, helping researchers choose the most efficient protocol. AI can analyze electronic health records (EHRs) to identify patients most likely to meet trial inclusion criteria, improving patient matching and recruitment efficiency. AI models can predict which patients are more likely to drop out of a trial, allowing researchers to proactively address potential issues and improve retention rates. AI can identify high-potential recruitment areas based on demographics and access healthcare facilities. AI can analyze historical data to more accurately estimate the required sample sizes, potentially reducing the number of participants needed. It can enable real-time adjustments to clinical trial parameters such as sample size or treatment arms based on interim data analysis, leading to faster and more accurate results. It can detect errors and inconsistencies in clinical trial data, improving data quality and reliability. AI algorithms can flag potential safety concerns early on, allowing for timely interventions.[23-28]

Applications of AI in drug discovery

- Target identification and validation
- Drug screening and lead discovery
- Drug optimization and design
- Preclinical and clinical development

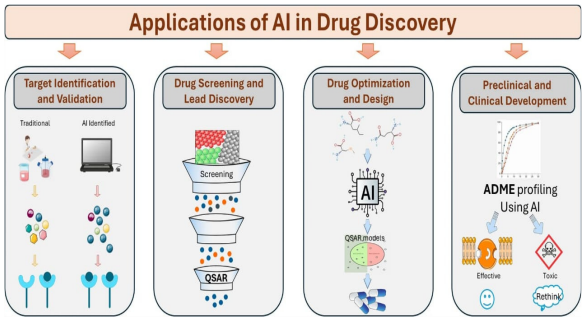

Fig:5 Applications in Drug Discovery

- **Target identification and validation**

AI significantly enhances drug target prediction by analyzing diverse biological data. AI algorithms can identify novel targets more effectively than traditional methods by integrating genomics, proteomics, and other sources. For example, AI can analyze genomic data to identify genetic variations associated with diseases and identify genes and their encoded proteins as potential targets. Similarly, AI can analyze proteomic data, such as protein structures and interactions, to identify proteins involved in disease pathways and assess their druggability. Furthermore, AI can integrate multiple data sources such as DrugBank PubChem, Antibiotic Combination DataBase (ACDB) , Antibiotic Adjuvant DataBase (AADB) as well as clinical trial data and electronic health records, to identify potential targets and predict their therapeutic potential.ML algorithms, such as DL and NLP, are crucial for

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analyzing complex datasets and identifying patterns and relationships that may not be readily apparent to human researchers

- **Drug screening and lead discovery**

AI-powered virtual screening and in silico approaches have revolutionized the identification of potential lead compounds for drug discovery. These methods utilize computational techniques to rapidly evaluate vast chemical libraries, significantly accelerating the process and reducing costs compared with traditional high-throughput screening.
ML algorithms are essential for these methods. For instance, they can be used to create quantitative structure–activity relationship (QSAR) models, that predict the biological activity of compounds based on their chemical structures. These models can then be used to screen large chemical libraries and prioritize compounds with the highest probability of binding to the target of interest. These AI-driven approaches have the potential to significantly accelerate the identification of promising lead compounds and ultimately improve the success rate of drug development

- **Drug optimization and design**

AI-driven techniques are revolutionizing drug development by optimizing critical properties, such as solubility, stability, and bioavailability. ML algorithms can analyze vast datasets of chemical structures and their associated properties to predict crucial parameters with high accuracy. For example, In QSAR predictions, approximately 1000–5000 data points were used for water solubility predictions whereas DL models can be used to predict drug stability under various conditions. For the protein function prediction task, researchers can leverage two open databases—the UniProt Consortium and the Protein Data Bank (PDB)—to gather protein sequence data from various species. This data can then be used to train prediction models through processes like batch downloading, data cleaning, and pre-processing. These predictive models enable researchers to rapidly identify and optimize drug candidates with improved physicochemical properties, thereby increasing their chances of successful clinical translation. Furthermore, DL algorithms, such as generative adversarial networks (GANs), can be used to generate novel chemical structures with desired properties, thereby expanding the chemical space explored in the drug design process

- **Preclinical and clinical development**

Predictive modeling of pharmacokinetics (PK), pharmacodynamics (PD), and toxicity profiles are crucial for efficient drug development. AI techniques, particularly ML, have advanced these capabilities significantly.
ML algorithms can analyze vast datasets of chemical structures and their associated PK/PD properties to predict key parameters such as absorption, distribution, metabolism, excretion (ADME), and drug-drug interactions. For example, DL models can accurately predict drug absorption across biological membranes, while other models can simulate drug distribution within the body.
Furthermore, AI can be used to predict drug reactions and toxicity profiles. ML algorithms can identify patterns and relationships between chemical structures and toxicity endpoints, enabling researchers to prioritize safer drug candidates and minimize the risk of unexpected side effects.[29-34]

Challenges and Limitations

Despite its transformative potential, AI faces several challenges in pharmaceutical research:
1. Data Quality and Availability: AI models require large, high-quality datasets, but inconsistencies in data sources can affect predictive accuracy (Ching et al., 2018).
2. Regulatory and Ethical Concerns: The use of AI in drug development raises ethical issues related to data privacy, bias in algorithms, and regulatory approvals (Topol, 2019).
3. Integration with Existing Systems: Adopting AI driven approaches requires significant investment in infrastructure, training, and system integration (Esteva et al., 2019).
4. Interpretability and Transparency: Many AI models, particularly deep learning algorithms, function as "black boxes," making it difficult to interpret their decision-making processes.[35-38]

Future of AI in Drug Discovery: Next Generation Innovations

The future of AI in drug discovery and development is promising, with ongoing advancements in quantum computing, federated learning, and AI-driven automation. 26 Collaborative efforts between pharmaceutical companies, regulatory bodies, and AI researchers will be essential in overcoming challenges and ensuring responsible AI implementation.24 As AI continues to evolve, its role in precision medicine, real-time drug monitoring, and automated clinical trials will further revolutionize the pharmaceutical industry

- **Quantum computing for drug design**

Quantum computing has the potential to revolutionize drug discovery by simulating molecular interactions with unprecedented accuracy. Unlike classical computers, quantum computers can process complex calculations exponentially faster, enabling precise modeling of drug protein interactions.

- **Self-Supervised learning for biomedical research**

Self-supervised learning (SSL) is a rapidly growing AI technique where models learn from large unlabeled datasets. SSL is particularly useful in biomedical research, where labeled data is scarce. By leveraging SSL, AI models can autonomously extract meaningful patterns from molecular structures, genetic sequences, and clinical trial data.[39-40]

Conclusions

AI offers significant advantages in addressing the challenges of classical drug discovery and development. AI can analyze large datasets for target identification, optimize chemical leads, and improve efficiency in virtual screening. It also aids in early clinical trials by enhancing patient recruitment and predicting outcomes to reduce trial failures. In personalized medicine, AI can help discover the difference between simple prognostic biomarkers and those that predict patient responses to treatments, streamlining cancer therapy development and improving success rates. However, there are still limitations that cannot be improved with the use of AI. For instance, AI

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cannot help to predict the use of inadequate preclinical models used in preclinical research. Many preclinical assays do not accurately represent the complexities of human tumors. As a result, some drugs that perform well in simplified models fail when tested in more complex human systems . This has been clearly observed with immune oncology agents.

In summary AI can be a highly valuable tool if correctly applied to several of the drug discovery and development processes. However, integration with current models will be challenging and time consuming; with the incorporation of multitasker teams, AI tools could boost the drug development process.

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