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Original Article

Artificial intelligence in drug discovery and development

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ABSTRACT

Artificial Intelligence (AI) has emerged as a transformative force in drug discovery and development, addressing challenges such as high costs, lengthy timelines, and frequent failures in pharmaceutical research. AI-driven approaches, including machine learning, deep learning, and bioinformatics, are revolutionizing various stages of the drug development process—from target identification and lead optimization to clinical trials and regulatory approval. AI enhances drug bioactivity prediction, facilitates personalized medicine, and streamlines clinical trial recruitment, improving efficiency and accuracy. Leading pharmaceutical companies are integrating AI to accelerate innovation and optimize therapeutic outcomes. Despite its vast potential, AI in drug discovery faces challenges such as data privacy, algorithmic bias, and regulatory hurdles. This review explores AI's applications, benefits, limitations, and future prospects in pharmaceutical research, highlighting its role in reshaping modern medicine.

Keywords: Artificial Intelligence, Drug Discovery, Machine Learning, Pharmaceutical Research, Clinical Trials, Bioinformatics

INTRODUCTION

The term "artificial intelligence" was given by John McCarthy at the Dartmouth Convention in 1956 to describe "the science and engineering of intelligent machines"[1]. The pharmaceutical industry conducts drug research, development, production, and distribution. The pharmaceutical value chain begins with drug discovery, the process of identifying novel therapeutic candidates. During the drug development process, a drug candidate undergoes preclinical study before becoming a clinically meaningful drug. Clinical trials are undertaken to ensure safety, efficacy, dose, and tolerance [2]. If the clinical study is deemed substantial and successful, the pharmaceutical company will submit a new drug application (NDA) to the regulatory body for approval after a thorough assessment of the findings. Drug discovery is costly, time-consuming, and frequently unsuccessful. Molecules typically take 10-12 years from discovery to market[3]. Enhanced treatments that offer incremental improvements over current medications are crucial, as they can enhance aspects of existing drugs like effectiveness, safety, tolerability, or convenience. However, these improvements typically do not involve alterations to biological targets that differ from those directly impacted by the existing therapies[4]. Artificial intelligence is commonly utilized in healthcare for the following purposes:

- Research
- Digital health monitoring and diagnostics
- Patient data & risk analysis
- Surgery
- Mental health
- Hospital Management
- Virtual assistant
- Drug discovery
- Wearable.

Principle Of AI

Life-science problems can be solved by any method or technology that offers conventional statistical, mathematical, and veterinary methods that are ineffectual or inefficient[5]. Information management, AI machine learning, and multi-agent systems can all significantly impact how experiments are carried out[6]. Technical assistance for integrating and

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developing human and robot capabilities can be obtained from the domains of agencies, natural language processing, vision, syntax, and human-computer interface[7]. The foundation for accessible discovery papers and the ranking of bioactive compounds according to their effectiveness as drug-like leads and the intended pharmacological effects are provided by machine learning[8]. These days, new fields of protein design application and biological target discovery are developing. Chemocentric techniques have become widely used in numerous molecular informatics machine learning systems[9].

AI in the lifecycle of pharmaceutical products

Given that AI can support logical medication design, its involvement in the pharmaceutical product development process from the bench to the bedside is conceivable[10].

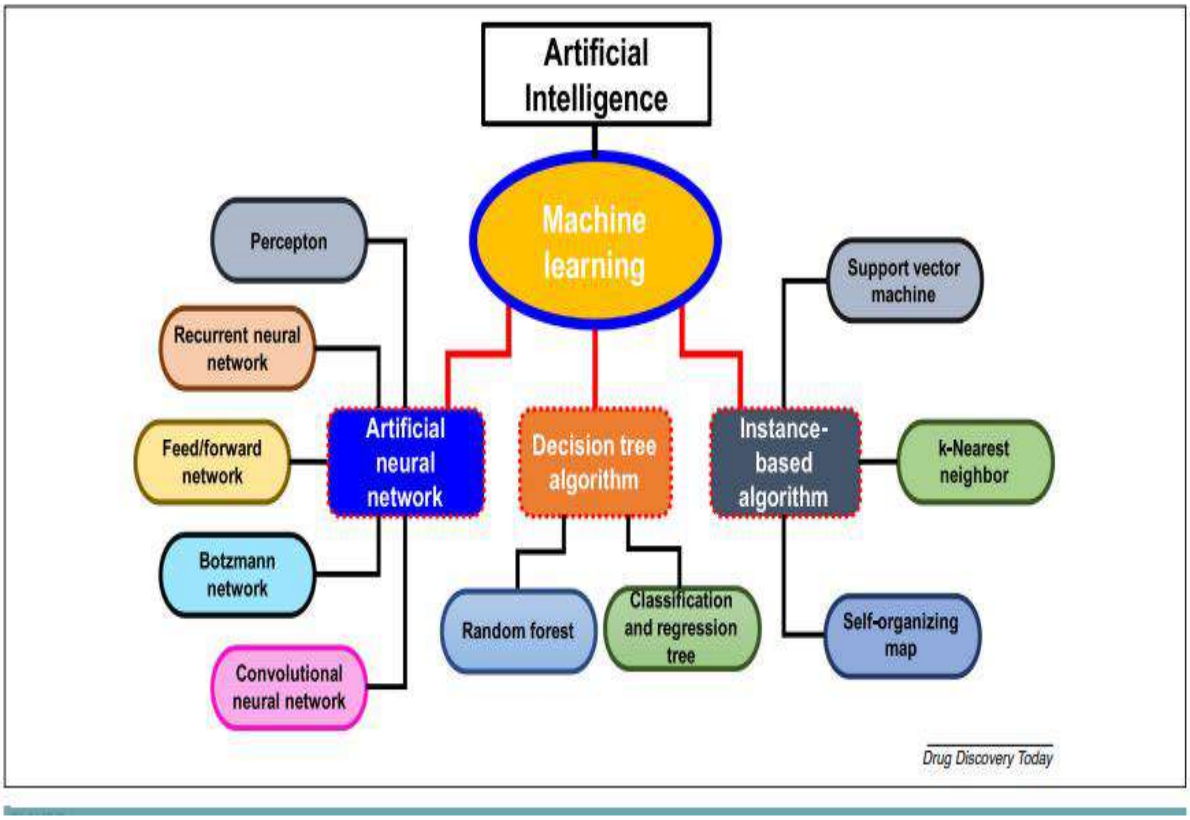

Figure-1.

Function Of AI

Artificial intelligence holds remarkable potential for growth in the biopharmaceutical sector. Presently, leading biopharmaceutical firms are utilizing various AI programs, including:

• **Mobile application aimed at enhancing health results:** The ability to recommend patients and improve patient outcomes through real-time data collection.

• **Personalized medicine:** The capacity to use a cloud-based technology to analyze vast amounts of patient data and find treatment choices.

• **Acquisitions galore:** Artificial intelligence and healthcare are being combined by new startups to meet the startup demands of big biotech enterprises.

• **Drug discovery:** Pharma companies in association with software companies are trying the most advanced technology forthe cutting cost and extensive process of drug discovery[11].

Drug Development Process :

The lengthy and intricate process of drug discovery can be broadly categorized into four areas:

• Target selection and validation
• Compound screening and lead optimization

- Preclinical studies
- Clinical trials[6].

First, the target of a specific disease must be determined. This requires cellular and genetic target evaluation, genetic and proteomic analysis, and bioinformatics assays. After that, the next step means identification, where computers are identified from libraries of molecules through using some of the methods such as chemical synthesis, high-throughput, and virtual screening. In silico studies are used in the iterative cycle to improve the functional properties of newly synthesized drug candidates in combination with structure-function and cellular functional assays. Subsequently, in vivo studies like pharmacokinetic investigations and toxicity tests are performed in animal models [8]. Finally, a drug candidate, who has successfully completed all preclinical tests, will be given to patients in a clinical trial. This step is characterized by three stages that require the drug to pass through them in succession. Phase I, includes the safety assessments of the drug on the small number of subjects; Phase II, includes the efficacy of assessments drug with a small number of people who are affected by the targeted disease; and Phase III, efficacy studies with a larger Phase III, effectiveness research using a more extensive number of subjects. Once the safety and efficacy of a drug candidate are confirmed at clinical stages, the area is reviewed by organizations such as the FDA for approval and operation shown in Fig.1[12,13].

Table 1: Approaches of Artificial Intelligence

DRUG DISCOVERY PROCESS	DRUG DESIGN TOPICS	AI MODELS
Target identification and study	Prediction of protein folding and Proton pump inhibitors (PPIs)	CNN: predicting the residue contact and FD/DCA: detecting druggable PPI sites
Hit discovery	Drug repurposing	Network pathology
	Virtual screening	SVM, AAE
	Activity scoring	SVM, RF, 3D graph CNN
Hit lead	QSAR	Traditional machine learning, DNN
	De novo design	Deep reinforcement learning, VAE, AAE
Lead optimization	Evaluation of ADME/T properties	CNN, multitask neural network

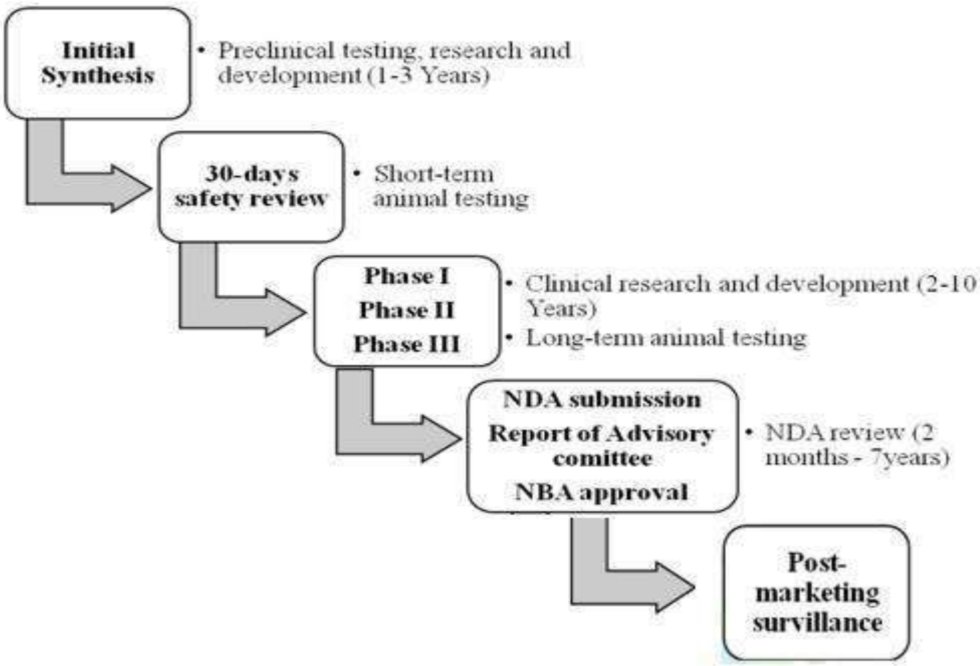

Figure 2: drug development process.

Clinical Research: AI and big data technologies work well together because AI can assist in synthesizing and analyzing ever-increasing amounts of data [14,15,16].

APPLICATIONS:

By examining social media and medical information, AI can find appropriate cohorts for clinical studies. AI technology can be used to notify patients and medical personnel about trial opportunities and streamline entrance requirements to make them easier for potential participants to access, which will speed up the recruiting process[17].

Disease Diagnosis: Additionally, the AI methods are the most effective in diagnosing various disease types. The use of artificial intelligence (AI) in healthcare provides previously unheard-of opportunities to improve patient and clinical group outcomes, reduce expenses, etc[18,19,20].

AI Applied in Top Companies in the Word: Over the past five years, the use of AI in the biotech and pharmaceutical sectors has fundamentally altered how scientists study illness, create novel medications, and more[21,22,23].

1. **Pfizer:** Immune Oncology.
2. **Roche:** Diabetic Macular edema.
3. **Johnson Johnson:** Stroke-Related Death, Merck & Co. MSD: Diabetes & Cancer Prevention Focus.
4. **Sanofi:** Repurposing drugs finds new use for some of its clinically potent molecules in genetic diseases.
5. **Glaxo Smith Kline**: Drug Discovery includes an in-silico drug discovery section and an artificial intelligence team.
6. **Amgen:** GNS health care medical research using precision medicine.
7. **Gilead Sciences:** April 2019: Drug Discovery.

Application of AI in Pharmacy:

1. Research development.
2. Diagnosis.
3. Drug development.
4. Disease prevention
5. Epidemic prediction.
6. Remote monitoring.
7. Manufacturing.
8. Marketing.
9. Personalized medicine and rare disorders.
10. Processing biomedical and clinical data.
11. Identifying clinical trial candidates.

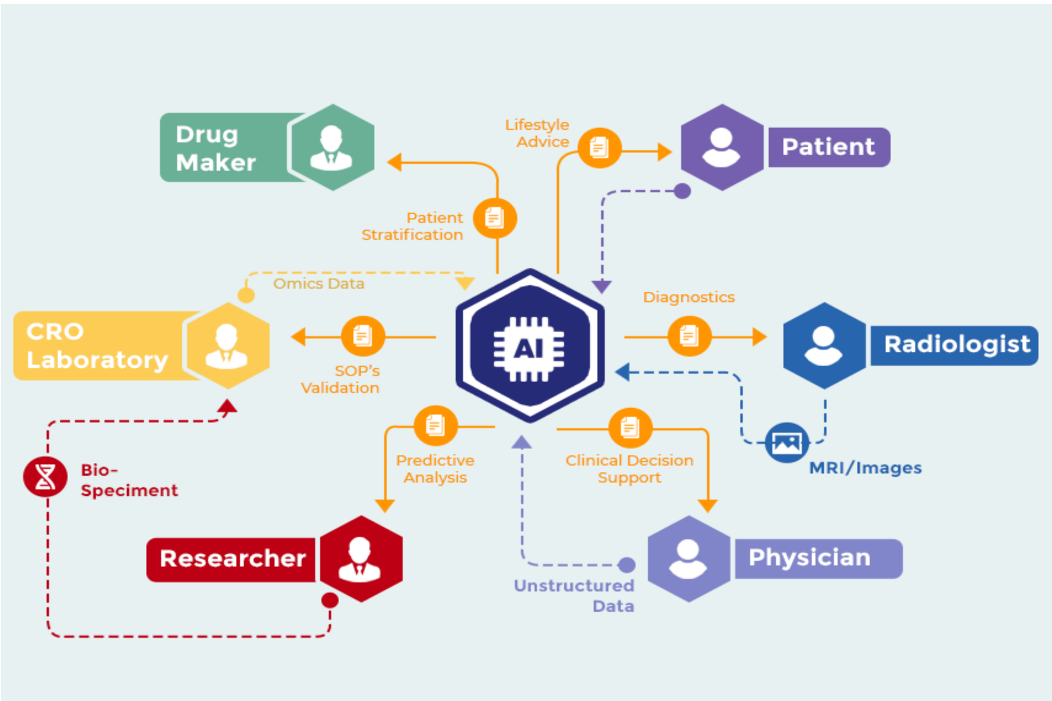

Fig. 3: Application Of AI[24].

Drug bioactivity prediction:

In actuality, the absence of bioactivity in many medications made from natural ingredients renders them ineffective. As a result, drug bioactivity evaluation is now a focus of drug discovery. Despite their ability to replicate the actions of molecules in the human body, in vitro and in vivo investigations are nevertheless costly and time-consuming. AI approaches have been successfully used to forecast pharmacological bioactivities, such as antiviral, antibacterial, and anticancer activities, because to their cost-effectiveness and time economy[25,26,27].

Review

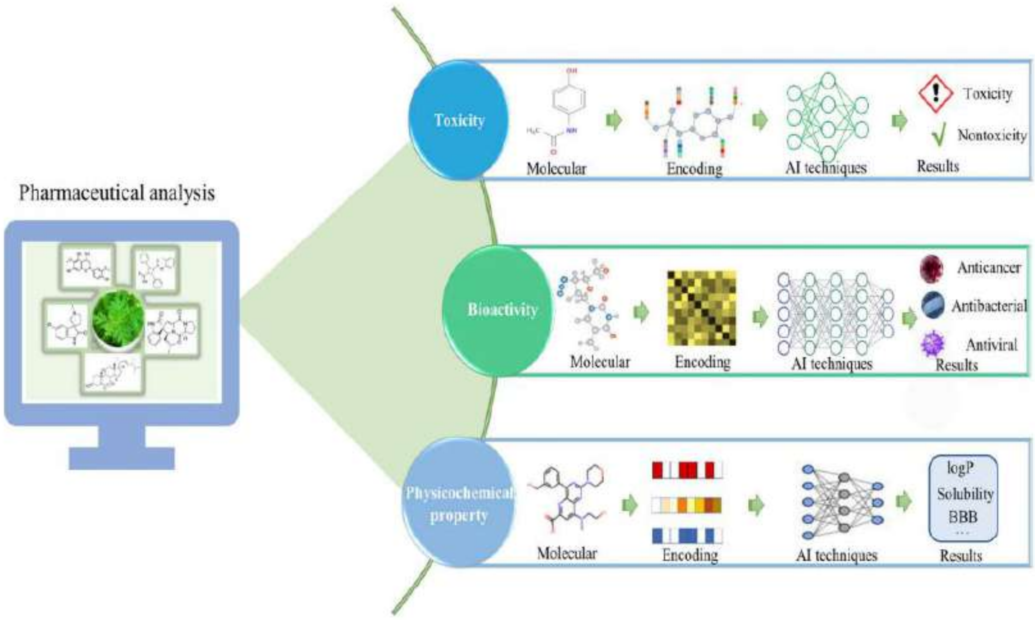

Figure 4. Application of AI techniques to pharmaceutical analysis.

Machine learning-based approaches:

Because illness mechanisms are intricate, it can be difficult to use a data-driven method to derive broad patterns of disease targets. Notwithstanding this challenge, a number of groundbreaking studies have demonstrated the potential effectiveness of applying machine learning approaches to drug-target identification and the ability to identify disease target patterns without the need for prior knowledge of biological dependencies. Ferrero and associates[28]. developed classifiers that forecast if a gene is a target or non-target of a medication. They used gene-disease association data from the Open Targets platform to build four classifiers: Random Forest (RF), Support Vector Machine (SVM), Neural Net, and Gradient Boosting Machine (GBM). They evaluated the significance of the input attributes for target identification using five different data types: route, animal model, genetic association, RNA expression, and mutation. They discovered that four classifiers performed similarly, with an AUC of 0.75 and an accuracy of about 70% . Mamoshina et al. [29]

Table 2. Quantity and description of curated databases for target identification

Database	Description	Quantity
DisGeNET [25]	A discovery platform of human-disease associated genes and variants with homogeneous annotation	628 K gene-disease associations, 17 K genes, 24 K diseases, 210 K variant-disease associations
Comparative toxicogenomics database (CTD) [26]	Comprehensive database for environmental effects on human health. It curates associations among chemical, gene, disease, phenotype, and exposure.	27 M gene-disease association
LinkedOmics [27]	Comprehensive database for molecular properties and clinical data of cancer. It collects multi-omics, clinical and Mass-spectrometry proteomics data of TCGA cancer.	13 K TCGA cancer samples
Open-Target platform [28]	A comprehensive database for target-disease association. It collects genetic and chemical data to aid target identification.	6.3 M association data with 27 K targets and 13 K diseases
DepMap portal [31]	A web portal providing cancer analytical and visualization tools. It contains genetic information and sensitivity of cancer cell lines.	Genetic characters of over 1 K cell lines
HMDD [30]	A database that collects miRNA-disease associations based on experimental evidence from PubMed papers	35 K miRNA-disease associations from 19 K papers
STRING [38]	A database of physical and functional protein-protein interactions	Total 3.1 B protein interactions
Therapeutic Target Database (TTD) [39]	A database of known therapeutic proteins, nucleic acids and targeted disease with related drugs.	3.4 K Targets and 37 K Drugs information

Devices Worked On Artificial Intelligence:[30]

1.Social media feeds (FB, TWITTER, INSTA)
2. Music and media streaming services.
3.Video games.
4. Online adds network.
5. Navigation and travel.
6. Banking finance.
7. Alexa.

AI in Science and Research:

AI is making lots of progress in the scientific sector. Large amounts of data can be handled and processed more quickly by artificial intelligence than by human minds.This makes it prefect for research where the sources contain high data volumes. AI is already making breakthroughs in this field[31,32,33,34].

AI in Cyber Security:

Another area that is benefiting from AI is cyber security. The risk of hackers is growing as more businesses move their data to cloud computing and IT networks.

AI in Data Analysis:

AI and ML have a lot to offer data analysis. Iteration allows AI algorithms to get better, which raises their accuracy and precision in proportion. AI can assist data analysts in managing and analyzing huge datasets.

AI in Transport:

AI has been used in the transportation industry for many years. Since 1912, airplanes have been guided through the air by autopilot. A plane's trajectory is managed by an autopilot system, which isn't exclusive to airplanes. Autopilot is also used by ships and spacecraft to assist them stay on course.

AI in Home:

In the guise of Smart Home Assistants, artificial intelligence has found a unique position in people's homes. Well-known smart home appliances like Google Home and Amazon Echo enable you to do a number of things using voice commands alone.

AI in Healthcare:

Because of its benefits, the medical industry is now utilizing this technology. Medical professionals and researchers are benefiting from AI in several ways[35,36].

Risks:

1. Automation-spurred job loss
2. Privacy violations
3. Weapons automatization
4. Deep fakes
5. Market volatility
6. Algorithmic bias caused by bad data
7. Socioeconomic inequality

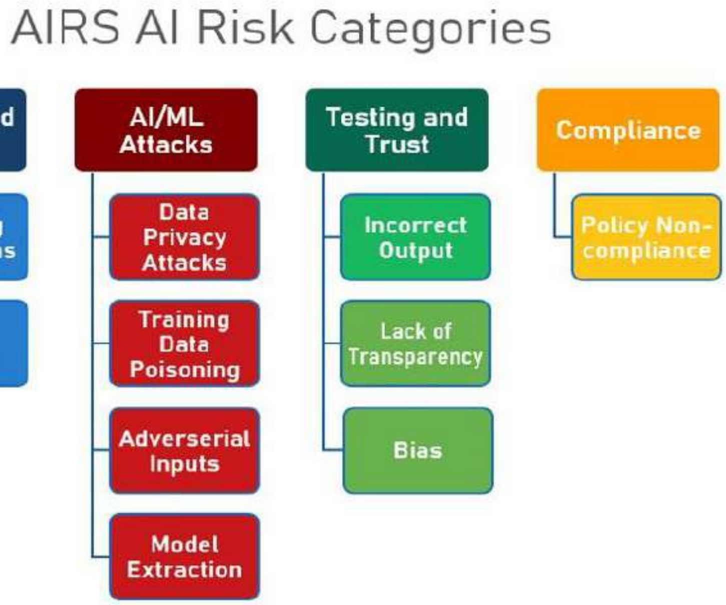

Fig. 8: Risk Of Artificial Intelligence [37].

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