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REVIEW ARTICLE

ARTIFICIAL INTELLGENCE IN PHARMACEUTICAL IN DRUG DISCOVERY: FROM STRUCTURE PREDICTION TO CADIDATE GENERATION OF NOVEL THERAPEUTICS

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ABSTRACT
The incorporation of artificial intelligence (AI) into drug discovery has fundamentally transformed the pharmaceutical landscape, creating exceptional prospects for expediting the development of novel therapeutics through the pathway from structure prediction to candidate generation. The flexibility and forecasting strength of AI have been effectively utilized throughout the drug discovery pipeline, encompassing target identification, accurate target structure prediction with AlphaFold and RoseTTAFold, virtual screening, compound screening, drug-target interaction analysis, and lead optimization for candidate generation. Through the application of machine learning, deep learning, and large-scale biological data, scientists can accelerate the identification of promising molecules, accurately predict three-dimensional protein structures, design novel therapeutic candidates via de novo and generative approaches, minimize human effort, and enhance therapeutic efficacy. This review presents a detailed overview of AI's contribution to drug discovery from structure prediction to generation of novel therapeutic candidates, emphasizing its applications in binding affinity prediction, ADMET evaluation, its benefits, and existing obstacles. It also outlines the present status of AI-driven drug discovery, its transformative potential, and key limitations to be resolved. Moreover, it examines forthcoming perspectives of AI in pharmaceutical innovation, including requirements for high-quality datasets, standardization, personalized medicine, and regulatory approval for novel therapeutic. Give me the 6 kwywords.

Keywords: *Artificial Intelligence (AI), Drug Discovery, Protein Structure Prediction, Machine Learning and Deep Learning Generative Drug Design, ADMET Prediction.*

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1. INTRODUCTION

It is estimated that 2.6 billion US dollars and over a decade of work are typically required in the field of drug discovery, but the success rate is very low due to high attrition rate.

Traditional drug discovery is a long process which includes target identification, hit identification, lead optimization, preclinical and clinical studies. This method has gaps like high cost, more time, trial and error and high failure rate.

This review focuses on discovery based on artificial intelligence and associated applications. We also highlighted the gaps present in the traditional method for drug designing. In addition, potential strategies and approaches to overcome current challenges are discussed [1].

To overcome these gaps, Artificial Intelligence (AI) is used in pharmacy. AI uses Machine Learning and Deep Learning to check millions of compounds in few hours. It uses tools like QSAR/QSPR, virtual screening, bioactivity and toxicity prediction to speed up the process.

The main concept of this review is from structure prediction to candidate generation of novel therapeutics. In this, first AI predicts the 3D structure of target protein using tools like AlphaFold. Then by virtual screening, drug-target interaction and de novo design, novel therapeutic candidates are generated.

Traditional drug discovery cannot perform tasks that only AI can do. Traditional method cannot predict accurate 3D protein structure without X-ray crystallography, cannot screen millions of compounds in a few hours, cannot accurately predict binding affinity and drug-target interaction before synthesis, cannot design novel molecules from scratch (De Novo Design), and cannot predict ADMET and toxicity at early stage [2]. These gaps cause high cost and 10-15 years of

time. Only AI can overcome these. AI using tools like AlphaFold predicts structure in minutes, uses virtual screening for high-throughput filtering, applies deep learning for binding affinity prediction, uses Generative AI for creating new chemical entities, and performs early ADMET/toxicity prediction. Thus, AI reduces cost, time and failure rate, which traditional method cannot achieve [3].

DRUG DISCOVEY PROCESS

Drug discovery is the process of identifying a new molecule that can become a medicine to treat a disease. It is a long, expensive, and high-risk process that takes 10-15 years.

1. Target Identification

The first step is to find the biological cause of a disease. Scientists identify a specific protein, enzyme, or gene that is responsible for the disease. This is called the Target.

2. Target Validation:

Scientists confirm that if we block or activate this target, the disease will be cured. This is tested in cells and animal models [4].

3. Hit Discovery

Thousands of chemical compounds are screened to find which one interacts with the target. This is done by High-Throughput Screening in the lab and Virtual Screening using Artificial Intelligence (AI). The active molecules are called Hits.

4. Lead Optimization

The Hit is not a perfect drug. Chemists modify its chemical structure to improve its potency, reduce its toxicity, and improve its properties like solubility and absorption. The improved molecule is called the Lead compound.

5. Preclinical Testing

The Lead compound is tested on animals to check its safety, toxicity, and ADMET properties (Absorption, Distribution, Metabolism, Excretion, Toxicity). If it is toxic, it fails here.

6. Clinical Trials (Human Testing)

This has 3 phases:

Phase I: Tested on 20-100 healthy volunteers for safety.

Phase II: Tested on 100-500 patients for efficacy and side effects.

Phase III: Tested on 1000-5000 patients on a large scale to compare with existing drugs.

7. Regulatory Approval

If clinical trials are successful, all data is submitted to regulatory authorities like USFDA and DCGI for approval. After approval, the drug is launched in the market [4, 5,6].

AI TOOLS AND TECHNIQUES IN DRUG DISCOVERY

Artificial Intelligence has made drug discovery faster, cheaper, and more accurate. AI can analyse huge amounts of data, predict drug behavior, and design new molecules which traditional methods cannot do easily.

A. Techniques of AI Used In drug discovery

1. Machine Learning (ML): It learns from old data to predict new results. Used for predicting drug activity and toxicity.
2. Deep Learning (DL): A part of ML using neural networks. Used for image analysis, protein structure prediction, and molecule generation.
3. Natural Language Processing (NLP): It reads scientific papers, patents, and patient records to find new drug targets. Ex: IBM Watson.
4. Generative AI (GANs & RL): Generates completely new drug molecules with required properties. Ex: ORGANIC tool.
5. Molecular Docking and Virtual Screening: AI checks how well a drug binds to its target protein on computer before lab testing.
6. QSAR Modeling: Quantitative Structure-Activity Relationship. It predicts biological activity of a compound from its chemical structure.

B. Ai Tools In Drug Discovery

1. AlphaFold: By Google DeepMind. Predicts 3D structure of proteins from amino acid sequence. Very useful for finding drug targets.
2. IBM Watson:Uses NLP to read patient reports and suggests personalized treatment for cancer.
3. DeepChem: Open-source Python library. Has MoleculeNet with 7 lakh compounds. Used for virtual screening and lead optimization.
4. DeepTox: Predicts toxicity of more than 12,000 compounds using deep learning. Removes harmful drugs early.
5. Atomwise (AtomNet): Uses deep learning for virtual screening of millions of compounds in hours.
6. BenevolentAI:Uses AI to find new uses for old drugs. Used during COVID-19 for drug repurposing.
7. Insilico Medicine (Chemistry42): Generates novel molecules using Generative AI [7].

8. ORGANIC: Creates new molecules using GAN + Reinforcement Learning.
9. Hit Dexter: Removes false positive compounds using Random Forest and AdaBoost models.
10. Delta Vina & Potential Net: Predicts binding affinity between drug and protein accurately [8].

ROLE OF PHARMACIST IN AI DRIVEN DRUG DISCOVERY PROCESS

1. Bridge: AI reads data fast but has no clinical sense. Pharmacist connects AI prediction to real patient care.
2. Target Validation: AI finds protein targets. Pharmacist checks if it is druggable and safe, not toxic to other organs.
3. Lead Optimization: AI designs 1000s of molecules. Pharmacist checks Lipinski Rule, solubility, ADMET, and drug-drug interactions. Suggests chemical changes if toxic.
4. Personalized Medicine:AI uses genes and age. Pharmacist reads CYP450 reports, selects right drug and dose to avoid ADRs, counsels patient. Useful in cancer, cardio.
5. Clinical Trials: AI finds patients from EHRs. Pharmacist verifies history, allergies, monitors ADRs, ensures GCP/USFDA compliance, does tele-counselling.
6. Drug Repurposing: Old drug for new disease. Ex: Remdesivir in COVID. Pharmacist decides dose and safety. Saves 6-7 years [9,10].

ADVANTAGES AND DISADVANTAGES

Advantages

1. Finds new life-saving medicines
2. Targets exact disease cause
3. Ensures safety through clinical trials
4. AI makes discovery faster, cheaper
5. Enables personalized medicine for patients

Disadvantages

1. Takes 10-15 years long time
2. Costs crores, 90% failure rate
3. Requires animal and human testing
4. AI needs costly computers, coding
5. Wrong data gives wrong results.

CONCLUSION

In conclusion, drug discovery is a long, costly and high-risk process that is essential for finding new life-saving medicines, and while traditional methods face problems of time, failure and ethics, AI tools like AlphaFold, DeepChem and DeepTox have made it faster, cheaper and more accurate; however, AI cannot replace laboratory testing and pharmacist expertise, so the best future is a combination of AI speed and pharmacist clinical judgment to deliver safe, effective and personalized medicines to patients.

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INFORM CONSENT AND ETHICAL CONSIDERATION

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