

## The Rise of Artificial Intelligence in Drug Discovery

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### ABSTRACT -

The current of artificial intelligence and machine learning has been significant. It has reduced the human workload improved quality life significantly. This article describes the use of artificial intelligence and Machine learning to agument drug discovery and Development to make them more efficient and accurate. In this study a systemic evaluation of studies was carried out these were selected based on prior knowledge of the authors and keyword search in publically available databases which were filtered based on related context, abstract methodology and full text. This body of work supported the roles of machine learning and artificial intelligence in facilitating drug development and discovery process, making them more cost effective or altogether eliminating the need for clinical trials, a wining to the ability to conduct simulations using these technologies. They also enabled researchers to study different molecules more extensively, without any trails.

**Keywords:** Artificial intelligence, drug discovery AI- assited content generation AI-limitations

### I. INTRODUCTION

One of the key application of AI in medicinal chemistry is the prediction of the efficacy and toxicity of potential drug compounds. Classical protocols of drug discovery often rely on labor intensive and time-consuming experimentation to assess the potential effects of a compound on the human body.

In the Pharma Space, AI is working with researches to supports the decision – making process for existing drugs and expanded treatments for other conditions, as well as expediting the clinical trials process by finding the right patients from several data sources.

Artificial Intelligence (AI) is Transforming many areas of science and drug discovery is no exception. AI is increasingly being used in the process of drug discovery which is defined as the process of designing, testing and developing new drugs to treat various diseases. The use of AI in drug discovery is a relatively new approach that has the potential to significantly

accelerate the process and improve the succes the rate of bringing new drugs to the market. AI algorithms can screen millions of drug candidates in a matter of hours, which is a game changer compared to traditional drug development methods that can take years of testing and and analysis.

This has led to an increasing interest and investment in the use of AI in drug discovery as it brings a more efficient and cost-effective approach to the development of new drugs.

### Advantages Of Artificial Intelligence In Drug Discovery –

1)AI for drug discovery plays crucialrole in enhancing the accuracy and efficiency of various quality assurance processes in the domain of drug quality control.

- 1) AI can aid in predicating drugs bioactivity by leveraging machine learning algorithms to analyze vast amounts of data on known compounds and their biological activities.
- 2) These algorithms can learn from this data to predict the bioactivity of new, untested compounds
- 3) One of the most significant is increased efficiency speed.

### Disadvantages of AI in drug discovery :-

- 1) Expensive – the launch of AI causes huge money consumption. Complex designing of the machine maintance and repair are highly cost-effective.
- 2) No replicating Humans – Robots with AI technology are associated with the power of thinking like humans & being emotionless.
- 3) No important with experience : Human resources can be improved with experience.
- 4) No original creativity : Machine with AI technology have neither sensitivity nor emotional intelligence.

### Applications of Artificial Intelligence in Drug Discovery :-

- 1) Faster drug development
- 2) More effective drugs
- 3) Better clinical trial design

- 4) Prediction of drugs bioactivity
- 5) AI in quality assurance
- 6) Drug repurposing
- 7) Patient Stratification

#### Genetic Algorithms (GA) in drug discovery :-

- 1) Genetic algorithms (GAS) are type of evolutionary algorithms, inspired by the process of natural selection that have been widely employed in drug discovery to explore large chemical spaces and identify promising lead compounds.

#### Principles of Genetic Algorithms

- 1) Population – GAs work with population of candidate solution (molecules) represented by chromosomes.
- 2) Fitness Function – each candidates is evaluated using fitness function that scores its potential as a drug.
- 3) Selection – The fittest candidates are selected to contribute to the next generation.
- 4) Crossover – Genetic Material is exchanged between selected candidates to create new offspring.

#### Knowledge Based Systems (KBS) in drug discovery –

- 1) A knowledge-based system (KBS) is a computational approach that captures and uses knowledge from variety of sources.
- 2) Knowledge base (K.B.) is a data base to knowledge, information related to any particular topic is stored in the form of fact bases and the relations between various factual data points in fact bases
- 3) When the data from FB & RB are efficiently interpreted with the help of inference engines, the entire system is known as an expert system.
- 4) Currently a knowledge based system is a major area of artificial intelligence with can help in making decisions based on the data and information that resides in their database.

#### Limitations of AI in drug discovery –

- 1) Lack of domain expertise :- AI requires extensive training on specialized datasets and drug discovery datasets are often limited and complex.
- 2) Black box models - Many AI models used in drug discovery are black boxes meaning it is difficult to understand how they make their predictions.

- 3) Overfitting and Bias – AI models can overfit to training data resulting in poor performance on unseen data.
- 4) Limited generalizability – AI models are often trained on specific datasets and tasks and may not generalize well to different datasets.

## II. CONCLUSION -

Many attempt are being made in applying AIDD. The results need to be judiciously applied. The AIDD models are only as good as the Training Provided to them. If sufficient reliable data is provided during training, we can trust the Model. Hence it is important to pay attention to data quality before taking up the AI model development.

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