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A Review Article on Artificial Intelligence in Drug Discovery & Development

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ABSTRACT

Artificial intelligence has many effective uses, ranging from language prediction to advancements in the pharmaceutical industry, and it speeds up and lowers the price of drug discovery and development. As the amount of drug-related data grows, the deep-learning method has been applied at every stage of the drug discovery process. I provided a general overview of artificial intelligence (AI) and its use in drug research and discovery in this mini-review. ligand-based quantitative structure activity and property, computers to assist drug discovery, De Novo drug design, integration with single cell technology, drug metabolism, and excretion; recent developments in tooth loss and colorectal cancer; the combination of plant-based traditional remedies; and demonstrating an AI-assisted platform used to discover the serotonin 5-HT1A drug, which will enter clinical trials in less than a year.

INTRODUCTION

The pharmaceutical sector is undergoing a fundamental change in drug determine and growth .all grateful to unification of artificial intelligence [AI]. Innovation of the artificial intelligence technique has achieved great improvements in different sectors, particularly biological technologies, to lower the drug research and development cost and time and failure-rate procedures.
Drug discovery scientists found it difficult to create an efficient system that would deliver therapeutic agents to the intended target while minimize their side effects and maximize their capability Additionally, developing novel therapeutic agents requires more time, effort, and money; therefore, classical computer approaches, such as molecular grounding and Virtual Screening, is used as an different to get around those restrict. Their inaccuracy and ineffectiveness highlight the new methods to overcome those barrier.

Extensive drug discovery action is estimated take 12 years, beginning with preclinical trial like Hit and leading invention and improving and continuing phase I, II, and III clinical trials before final drug approval used in humans. Entire process is expensive, costing about 1.2 billion dollars, and is complicated by the drugs that are taken off the market because of their negative effects on humans. Thus, a complex system like Artificial Intelligence, which includes Deep Learning and Machine Learning, has effectively speed up and reduced the cost of the drug development process.

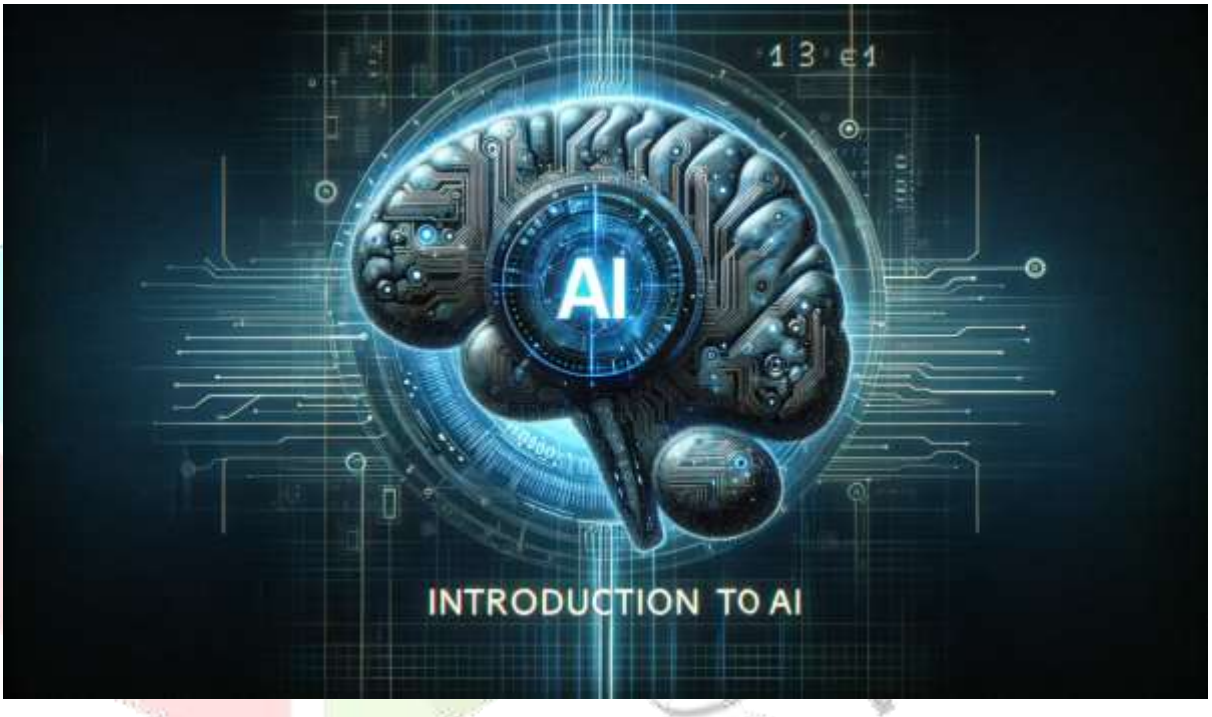
AI is going to transform drug discovery. The biggest obstacle to launching a novel medication is the time and expense needed to test it on patients before its effectiveness is determined. AI's primary contribution to drug discovery is the selection of tests with the highest likelihood of success, which reduces risk in the process as it is incorporated into more and more processes.

The pharmaceutical business has begun to utilize AI at a surprising rapid speed. AI systems are known to make predictions quickly yet inaccurately. The pharmaceutical industry's emphasis on safety is in conflict with this to the extent that it exists. Indeed, it hasn't been successful to bring AI right to the patient's bedside (Herper, 2017). AI predictions can be verified through trials prior to patient involvement, provided that it remains within the parameters of the research and development process

Large pharmaceutical corporations discovered a novel way to reduce risk during the early stages of drug discovery: acquiring intriguing molecules from smaller biotech businesses through in-licensing. For these molecules, pharmaceutical firms paid more, while tiny

Businesses took on the risks associated with early discovery. The big businesses focused on their intensity, which are commercialization and expensive clinical trials. During the past ten years, this trend has escalated.

In conclusion, AI has completely altered the pharmaceutical zone by improving the clinical trial, enabling tailored therapies, and enhancing the skill the medical diagnostics.



EVOLUTION OF AI

You might be surprised to learn how old this technology is. Ancient Greek and Egyptian mythologies even contain stories about mechanical men. The turning points in AI history listed below outline the progress of AI from its inception to the present.

AI Maturation (1943-1952)

- In 1943, Warren McCulloch and Walter Pits completed the first piece of work that is today known as artificial intelligence. They put forth an artificial neuron model.

- 1949, Donald Hebb showed how to change the strength of the connections between neurons using an updating method. Hebbian learning is the current name for his rule.

- Alan Turing, an English mathematician, invented machine learning in the year 1950. In "Computing Machinery and Intelligence," Alan Turing presents a test he developed. The test, known as a Turing test, can determine whether the machine is capable of displaying intelligent behaviour comparable to that of human.

- In 1955, Herbert A. Simon and Allen Newell developed the "first artificial intelligence program," known as "Logic Theorist." 38 out of 52 mathematical theorems were proven by this program, and some theorems also had new, more elegant proofs found.

- McCarthy, an American computer scientist, coined the term "artificial intelligence" in 1956 during the Dartmouth Conference. AI was first introduced as a topic of research.

Early enthusiasm all over the golden years (1956-1974)

- In 1966, the researchers focused on creating algorithms that might resolve mathematical issues.
- In 1966, Joseph Weizenbaum developed the first chatbot, called ELIZA.

- The first intelligent humanoid robot, known as WABOT-1, was constructed in Japan in 1972.

The first AI winter (1974-1980)

- The period from 1974 to 1980, AI experienced its first winter. The term "AI winter" describes the period of time when computer scientists faced a severe lack of government funding for AI research.

  - Public interest in artificial intelligence declined during AI winters.

Artificial intelligence (AI) Development (1980-1987)

- In 1980, AI returned with "Expert System" following a period of hibernation. Expert systems were designed to mimic a human expert's decision-making process.

- Stanford University hosted the American Association of Artificial Intelligence's inaugural national conference in 1980.

The second (AI) winter (1987-1993)

- The second AI Winter period lasted from 1987 until 1993.

- Once more, the government and investors stopped supporting AI research because it was expensive but did not produce effective results. Expert systems like XCON were incredibly economical.

Intelligent agents came into being (1993–2011)

- In 1997: IBM Deep Blue defeats Gary Kasparov, the global chess champion, to become the first computer to defeat a world chess champion.
- In 2006: AI entered the business sector in Additionall, businesses like Netflix, Facebook, and Twitter began utilizing AI.

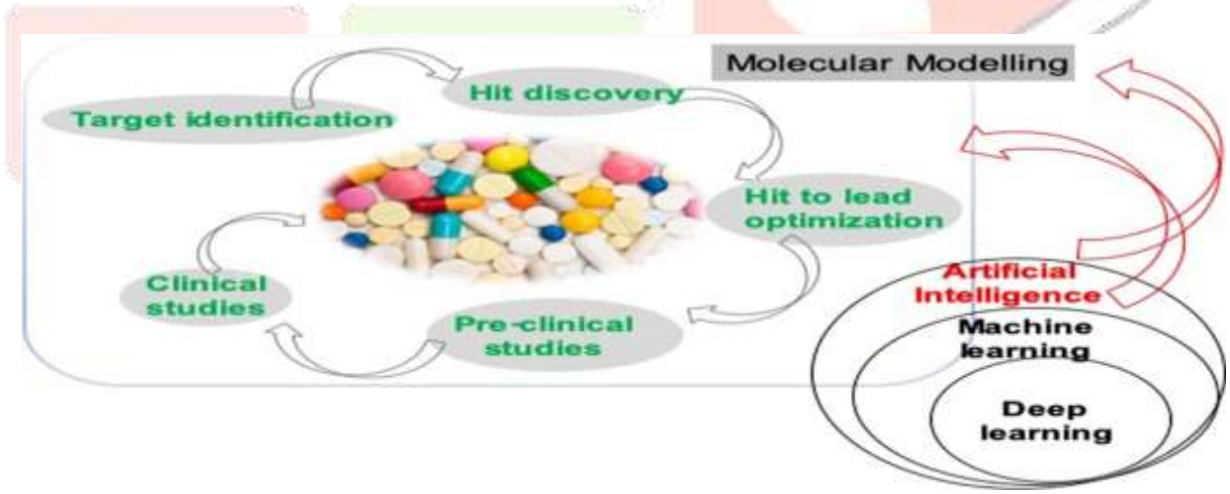
General intelligence, large data, and machine learning (2011–present)

- IBM's (2011) Watson was victorious in the quiz show Jeopardy, which required it to solve both challenging questions and riddles. Watson had demonstrated its ability to comprehend plain language and its speedy problem-solving skills.
- In 2012, Google released the function for its Android app,
- In 2014 saw the victory of the chatbot "Eugene Goostman" in the infamous "Turing test."
- In 2018: The IBM "Project Debater" fared remarkably well while debating difficult subjects with two expert debaters and performing correctly. This display advancement in natural language processing and ability of AI system to approach complex and delicate consultation.

Machine learning and deep learning applications of artificial intelligence

The process of transferring data, information, and human intelligence to machines is known as artificial intelligence, or AI. The development of autonomous machines with human-like thought and behaviour is the primary objective of artificial intelligence. These machines are capable of learning and solving problems to accomplish tasks and imitate human behaviour.Machine learning is a branch of AI that doesn't require clear programming. Algorithms are used in machine learning to examine data and identify patterns, which are subsequently used to inform decisions.

Deep learning models are more accurate than machine learning models, but they require more data and computational power. Machine learning models eventually cease getting better, while deep learning models can scale better with more data.



Impact of AI on Drug Discovery & Development

A. AI IN DRUG DISCOVERY

Historically, traditional drug development techniques have required a significant amount of work and resources due to their time-consuming and difficult nature. The process of going from concept to market frequently takes years or even decades. There have been numerous failures in this procedure, which is divided into phases including target identification, validation, lead compound recognition, effectiveness, and clinical trials. Traditionally, most promising medication candidates fail at different phases of development, especially in clinical trials, primarily because of safety or ineffectiveness issues. Additionally, these approaches have been hindered by their limited ability to analyse data, mostly depending on linear models and empirical data. Because biological data is complicated, such dependency has seriously restricted the ability to predict drug interactions, undesirable effects, and potency.AI in drug discovery is a quickly expanding and developing topic of study with the goal of improving the process's accuracy and efficiency. A number of phases of drug research, including target verification, molecular screening, lead effectiveness, and toxicity prediction, have seen the use of AI

in recent years. The capacity to evaluate the interpret massive quantity of biological data, pharmacological, proteomic, and genomic data, in order to find possible therapeutic targets is one of the main benefits of artificial intelligence in developing drugs In addition, virtual libraries of chemical compounds can be screened by AI algorithms to find possible therapeutic candidates that meet specified requirements.

B. FUNCTION OF DRUG DISCOVERY

It has demonstrated significant ability in accelerating up the drug discovery process and enhancing the accuracy as well as effectiveness of several phases of drug development. However, more study is necessary to solve ethical and legal issues as well as analyze and improve AI models for discovering new drugs. Research on artificial intelligence (AI) is crucial to the drug development process because it aims to create models that can transparently and clearly explain their judgments and predictions.

- Data Analysis
- Making Evidence-Based Decisions:
- Improved Design of Clinical Trials:
- Personalized Health Care
- Improved Regulation

C. INTERPRETABILITY ISSUE

One of the most important features of AI models for drug discovery is ability to be understood, which enables researchers to easily understand how AI algorithms are generating predictions and judgments. This can enhance the accuracy as well as reliability of AI models and offer significant insights into the biological processes supporting medications. To

Increase the understanding of AI models for drug discovery, a number of techniques can be applied:

- Model explanation:
- Features that are important:
- Model comparison:
- Human error:

Challenges of AI in Drug Discovery

The number of limitations that need to be taken in account, even with the possible advantages of AI in drug research. The Large amounts of data are usually needed for training in Artificial intelligence based methods. Quantity of available data are frequently restricted, the data may be incorrect and low quality, which might compromise the accuracy as well as reliability of the findings. Moral considerations pose an additional challenge because AI-based methods may give rise to questions regarding disadvantage and fairness. For instance, predictions made by an ML system may be unfair or erroneous if the data utilized in teaching it has been distorted or insufficiently representative. It is crucial to address the issue of ensuring the just and moral application of Artificial intelligence is creation of novel medicinal substances. Challenges that Artificial intelligence faces in the field of pharmaceutical medicine can be addressed the number of ways. The creation of artificial data to complement current databases is one method known as enhancing data. This can improve the quality and dependability of the outcomes by expanding the amount and variety of data accessible for machine learning (ML) algorithm training. Explainable (AI) techniques are an additional strategy that seeks to offer visible and understandable justifications for the predictions generated by machine learning techniques. This can improve comprehension of the fundamental ideas and assumption driving these projections and reduce fears about prejudice and equality in AI-based methods. Present-day AI-based techniques are unable to fill the place of conventional experimentation or the knowledge and abilities of human research. AI can only make assumptions on the evidence at hand; people researchers must then verify and explain what they have learned. However, the drug development procedure can potentially be improved by merging AI with conventional laboratory methods. By mixing AI's capacity to predict with knowledge and experience of human researchers, it is feasible to accelerate the manufacturing of newly medicine and modify the drug development procedure.

Collaboration between AI Company and Pharmaceutical industry

In order to create novel and efficient therapies for a variety of illnesses, cooperation among AI companies and the pharmaceutical sector is essential. They can develop strong algorithms and machine-learning algorithms to forecast the effectiveness of possible drug candidates and expedite the drug development process by pooling their expertise and prior experience. Because AI algorithms may be used to examine the data gathered during clinical research in order to spot trends and potential side effects of the pharmaceuticals under test, this partnership may also assist increase the precision and effectiveness of these studies. This can expedite the entire drug discovery phase and assist pharmaceutical corporations in making well-informed judgments about which therapeutic candidates they will pursue. Additionally, cooperation between pharmaceutical experts and AI company can contribute to better

Affordability and accessibility. Artificial intelligence (AI) can be used to find possible new targets for pharmaceuticals. This can improve our comprehension of disease mechanisms and lead to the discovery of new drugs through the identification of particular biomarkers or alterations associated with a specific illness. To train machine learning models that can be used to find new chemicals or pharmaceutical goals businesses are creating their own data sets, utilizing pre-existing data sets, and purchasing data sets created by other companies. A genetic testing corporation that gathered genetic information on roughly 10 million individuals (as of 2020) and obtained consent from clients to utilize hidden data for pharmaceutical research is one example of this type of data use for biopharmaceutical discovery.

Application of Drug Discovery & Development

Drug Design

Artificial Intelligence (AI) greatly speeds up the drug development schedule by improving the discovery of promising chemical compounds. By analysing a vast range of chemical combinations and forecasting their possible binding affinities, artificial intelligence (AI) has streamlined the process from concept to clinic. Finding tiny compounds that meet a number of important requirements is the foundation of medication design. These consist of appropriate biochemical and biological characteristics, pharmacologic efficiency, an acceptable security description, and the innovation required to protect intellectual property rights for economic viability. Traditional techniques have a number of difficulties, including expensive computing costs, unpredictable accuracy, and lengthy input times, even if computer tools have transformed drug design and the process leading to development.

AI in Polypharmacology

The field of drug discovery is changing dramatically, abandoning the old "one drug, one target" model in favor of polypharmacology, a method that investigates how medications interact with several targets. The ability to improve therapy efficacy and more thoroughly address the complexities of complicated diseases is what is driving this change. AI is essential to the development of polypharmacology because it makes it easier to analyze intricate biological data and identify possible polypharmacological possibilities. The use of polypharmacology stems from a sophisticated comprehension of the molecular complexities and disease processes. The combining of large databases, such ZINC, PubChem, and DrugBank, among others, has fueled this progress. These resources combine enormous volumes of information about chemical characteristics, interaction affinity, and molecular routes.

AI in Chemical Synthesis

In the field of drug discovery, chemical production sustainability and efficiency are crucial. This field has seen tremendous change as a result of AI's development, which has improved responses and produced remarkably accurate outcome predictions. The combination of chemical knowledge and AI technologies allows for the quick synthesis of intricate drug compounds, expanding the pool of possible therapeutic discovery.

AI in Drug Repurposing

Pharmaceutical repurposing, sometimes known as drug repositioning or retasking, is the process of finding novel therapeutic uses for medications that were formerly created to treat different illnesses. Compared to conventional drug discovery pipelines, this strategy has attracted a lot of attention since it offers the ability to speed up the action, save costs, provide pharmaceuticals to patients sooner. Highlights the main advantages and distinctions between conventional drug discovery methods and drug recycling techniques. Additionally, the substantial advantages and difficulties of drug repurposing are described.

AI in Virtual Screening

An essential computer technique in contemporary drug development pathways is virtual screening. It makes it possible to quickly assess enormous chemical libraries in order to find possible hit chemicals that could be effective against a particular biological target. Filtering and prioritizing compounds with desired biological activity from large small-molecule libraries usually entails a series of analytical procedures. Structure-based virtual screening and ligand-based virtual screening are the two primary types of virtual screening techniques.

AI in Pharmaceutical Analysis

A key step in the drug development process, pharmaceutical evaluation includes the authentication, determination, measurement, and purifying of chemical compounds.
Both qualitative as well as quantitative experimental techniques are its mainstays. Despite the excellent accuracy of these techniques, it is still quite expensive to screen new drug candidates from a wide range of natural compounds. On the other hand, computational approaches provide a more affordable option. As a result, in addition to conventional experimental techniques, AI technologies are being used more and more to improve pharmaceutical analysis. Gives an overview of the main uses of AI in analysis of medicines.

CONCLUSION

Drug discovery using AI is not a recent development. For many years, creating tiny molecule targets has relied heavily on machine learning. AI has recently and continuously advanced, enabling it to reduce costs and increase productivity in other aspects of the drug discovery process. Small biotechnology enterprises are experimenting with a variety of novel AI applications in addition to reducing molecules and toxicity prediction, which are previously mainstays of cutting-edge drug discovery processes. This is hastening the change in big pharmacy business strategy. These companies purchase trial-ready chemicals from outside sources rather than conducting all the research internally. Adopting AI successfully throughout the drug research pipeline should significantly reduce drug development costs, even though several necessary stages are still unclear. This would allow the industry to produce medications for patient groups who were previously thought to be far too small to warrant the cost. The change of the drug determine and growth workflow improving the human decision-making skills depend heavily on real-world machine learning and artificial intelligence presentation applications. To speed up the identification of lucrative drugs, deep learning in AI has been widely used in conjunction with Computer-Aided Drug identification (CADD) techniques.

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