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Revolutionizing Drug Discovery: A Review on Artificial Intelligence, applications and future directions

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ABSTRACT
Recently, artificial intelligence (AI) has begun to be applied more widely in many facets of society, with the pharmaceutical sector leading the way in this regard. This review emphasizes the significant application of AI in various pharmaceutical domains, such as drug development and discovery, drug repurposing, enhancing pharmaceutical productivity, clinical trials, etc., to mention a few. This reduces the human workload and expedites the achievement of goals. There is also discussion on the future of AI in the pharmaceutical sector, current obstacles and solutions, and the methods and instruments used to enforce AI.

I. INTRODUCTION

Artificial intelligence integrated drug discovery and development has accelerated the growth of pharmaceutical sector, leading to a revolutionary change in the pharma industry.

In the 21st century artificial intelligence (AI) has become an important area of re-search in virtually all fields: engineering, science, education, medicine, business, accounting, finance, marketing, economics, stock market and law, among others perceive + Analyze + React.[1]

AI is defined as intelligence exhibited by an artificial entity to solve complex problems and such a system is generally assumed to be a computer or machine.

Artificial Intelligence is an integration of computer science and physiology Intelligence in simple language is the computational part of the ability to achieve goals in the world. Intelligence is the ability to think to imagine creating memorizing and understanding, recognizing patterns, making choices adapting to change and learn from experience. Artificial intelligence concerned with making computers behave like humans.[2]

The pharmaceutical industry has seen a rapid rise in data digitization in the last several years. The difficulty of learning, evaluating, and using that knowledge to address intricate clinical issues, however, is a consequence of this digitization. Because AI can manage massive volumes of data with improved automation, this encourages its use.[3]

Tools and Network of Artificial intelligence:

AI encompasses a number of approach disciplines, including machine learning (ML), a foundational paradigm, reasoning, knowledge representation, and solution search. ML makes use of algorithms that are able to identify patterns in a collection of data that has undergone additional classification. Deep learning (DL), a branch of machine learning (ML), uses artificial neural networks (ANNs). These consist of a collection of interrelated, very advanced computing components that imitate the way electrical impulses are sent in the human brain by using "perceptons" that are comparable to biological neurons.[4]

An artificial neural network (ANN) is made up of a collection of nodes that receive individual inputs and, using algorithms to solve issues, convert them into output either singly or in many links. Recurrent neural networks (RNNs), convolutional neural networks (CNNs), and multilayer perceptron (MLP) networks are some of the different types of artificial neural networks (ANNs) that use either supervised or unsupervised training processes.

The MLP network can be used as universal pattern classifiers and is often trained using supervised training processes that only operate in one direction. Its applications include pattern recognition, optimization assistance, process identification, and controls.[5,6]

The networks that make up the fundamental architecture of AI systems have served as the basis for the development of several technologies. The International Business Machine (IBM) Watson supercomputer (IBM, New York, USA) is one example of a tool created with AI technology. It was created to help with the examination of a patient's medical records and their association with a large database, which led to the recommendation of cancer treatment plans. Rapid illness detection is another application for this technique. Its capacity to identify breast cancer in just 60 seconds served as evidence of this. [7]

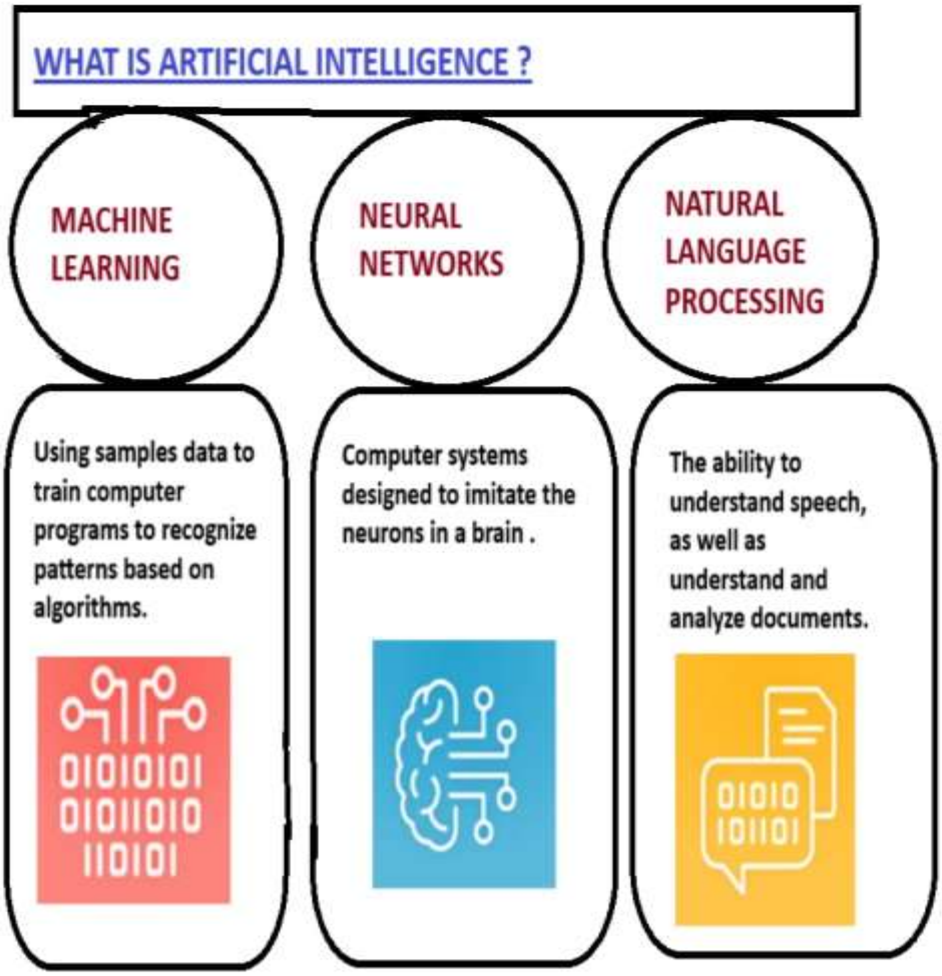

Figure 1.AI Tools and method domains

Machine Learning

Machine learning (ML) is a branch of artificial intelligence (AI) and computer science that focuses on the using data and algorithms to enable AI to imitate the way that humans learn, gradually improving its accuracy.[8]

A Decision Process: In general, machine learning algorithms are used to make a prediction or classification. Based on some input data, which can be labeled or unlabeled, your algorithm will produce an estimate about a pattern in thedata.

An Error Function: An error function evaluates the prediction of the model. If there are known examples, an error function can make a comparison to assess the accuracy of the model.

A Model Optimization Process: If the model can fit better to the data points in the training set, then weights are adjusted to reduce the discrepancy between the known example and the model estimate. The algorithm will repeat this iterative “evaluate and optimize” process, updating weights autonomously until a threshold of accuracy has been met.[9]

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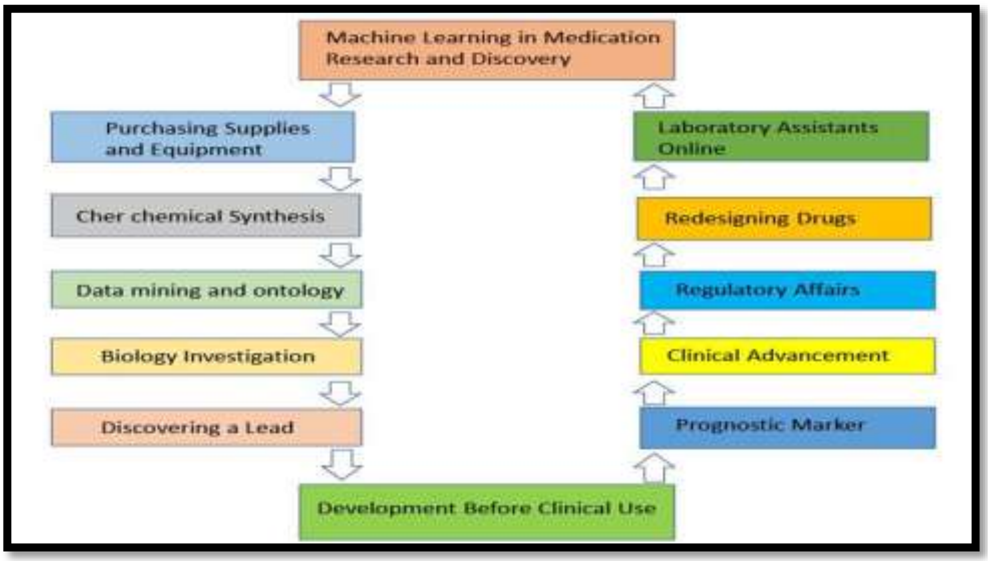

FIGURE2:-MACHINE LEARNING IN DRUG DEVELOPMENT AND DISCOVERY

Working Model of the Machine Learning

As per as the different types of machine learning is concerned, unsupervised Learning and supervised Learning played a central role. Supervised Learning explores the pattern within data to understand and recognize like groups within the given dataset. In contrast, supervised data used a set of input variables to predict the value of an output variable.

1.Unsupervised Learning: Unsupervised Learning uses the most common type of algorithm, called K-Means or Clustering. It is useful when it comes to identifying data structure.

2.Supervised Learning: It is the widely used machine learning algorithm, and it is the most common type of machine learning. It is also called Inductive Learning, including classification and regression. [11]

Applications of Machine Learning

Machine learning is being used widely, making the future more predictable. Recommendations we received from YouTube, Instagram, and Facebook are an application of Machine Learning. Other applications of machine learning are

1)Human Resource Information Systems: In short, it is also called an HRIS System, and it is used for identifying the best candidates for an open position using machine learning models to filter the applications.

2) Business Intelligence: In short, it is called BI. Machine Learning is used by vendors in their software to search potentially important anomalies and patterns of data points.[10]

3) Customer Relationship Management: The Machine Learning model used by the CRM software analyzes prompt sales members responding to important messages first and email.

Virtual Assistants: Smart assistants usually combine unsupervised and supervised learning machine learning models to decipher supply context and natural speech.[11]

Deep learning

Deep learning is a type of machine learning and artificial intelligence (AI) that imitates the way humans gain certain types of knowledge. Deep learning models can be taught to perform classification tasks and recognize patterns in photos, text, audio and other various data. [12]

An Artificial Neural Network is a network of collections of very simpleprocessors ("Neurons") each possibly having a (small amount of) local memory. The units operate only on theirlocal data and on the inputs, they receive via the connections or links which are unidirectional. A network unit has a rule forsumming the signals coming in and a rule for calculating anoutput signal that is then, sent to another network.[13]

Natural Language Processing (NLP)

NLPis an area of research and application that explores how computers can be used to understand and manipulate natural language text or speech to do useful things.

NLP researchers aim to gather knowledge on how human beings understand and use language

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so that appropriate tools and techniques can be developed to make computer systems understand and manipulate natural languages to perform the desired tasks.

The foundations of NLP lie in several disciplines, viz. computer and information sciences, linguistics, mathematics, electrical and electronic engineering, artificial intelligence, and robotics, psychology, etc. [14].

How does Natural Language Processing work?

Natural language processing (NLP) combines computational linguistics, machine learning, and deep learning models to process human language.[15]

Computational linguistics: Computational linguistics is the science of understanding and constructing human language models with computers and software tools. Researchers use computational linguistics methods, such as syntactic and semantic analysis, to create frameworks that help machines understand conversational human language. Tools like language translators, text-to-speech synthesizers, and speech recognition software are based on computational linguistics.[16]

Drug Discovery and Development

Drug discovery involves the exploration and analysis of various compounds that can enhance the well-being of patients and contribute to their improved quality of life by addressing disease symptoms or progression. The drug development timeline spans several years and can be plagued with failures and large resource expenditures.

However, there is also a great deal of learning that happens at each stage along the drug development timeline. This learning ensures that drug developers and drug manufacturers are bringing to market the right compounds, also called small molecules, with the correct safety profiles that will benefit the intended patient population.

Our drug development overview encompasses the entire journey of identifying, researching, and refining potential drug candidates. We touch on considerations for preclinical studies, clinical trials, regulatory approval, and post-marketing surveillance that are important to bring safe and effective medications to market.[17]

Artificial Intelligence in drug discovery and development

More than 1060 molecules make up the enormous chemical space, which encourages the synthesis of numerous pharmacological molecules [18]. AI can be used to address the time-consuming and costly medication development process that is limited by a lack of innovative technology [19]. AI has the ability to identify hit and lead compounds, validate drug targets more quickly, and optimize drug structure design. [20].Various uses of AI in drug discovery are illustrated in figure1

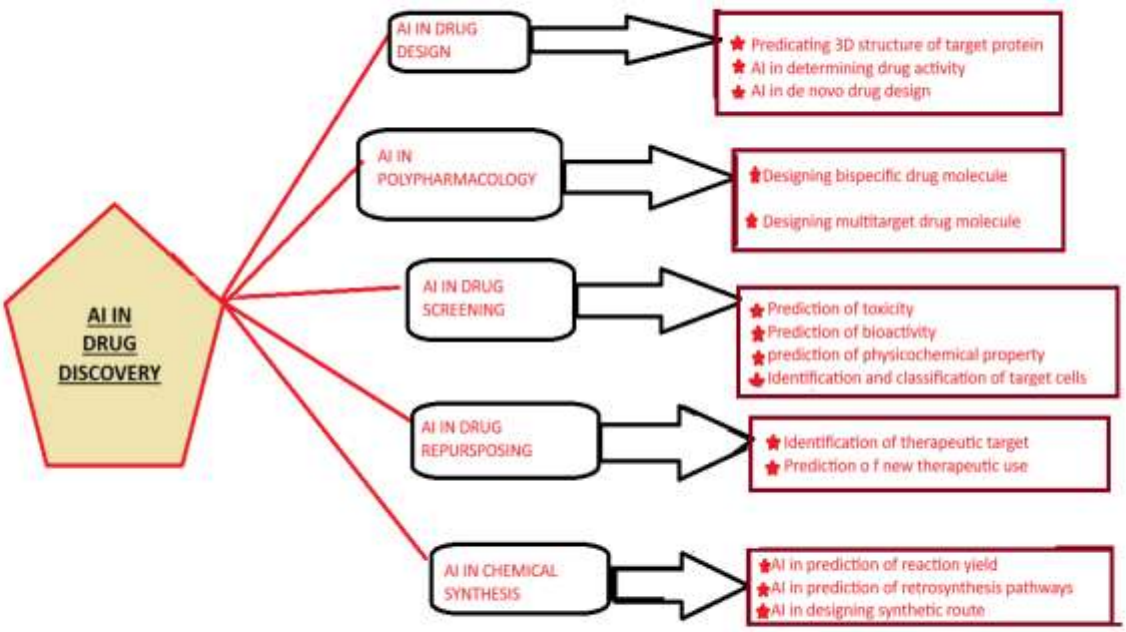

Figure 3.AI in drug discovery

Drug research and discovery are essential procedures that make it possible to address a wide range of medical issues. These procedures are expensive, time-consuming, laborious, and complex. From concept to testing, a number of challenges come up during the drug research process.

Technologies based on artificial intelligence enhance the pharmaceutical industry's capacity to find potent medications. This overview outlines the main difficulties that arise during the medication development and discovery processes, along with the ways in which artificial intelligence-based techniques are used to get past such difficulties and offer practical answers to health issues.

Drug discovery is a project motivated by the situation when there are no drugs for a disease or when existing drugs have limited efficacy and/or severe toxicity.

At the earliest stage, an underlying hypothesis needs to be developed that activation or inhibition of a target (e.g. an enzyme, a receptor, an ion channel, etc.) results in therapeutic
Effects for the disease, which involves target identification and target validation.[21]

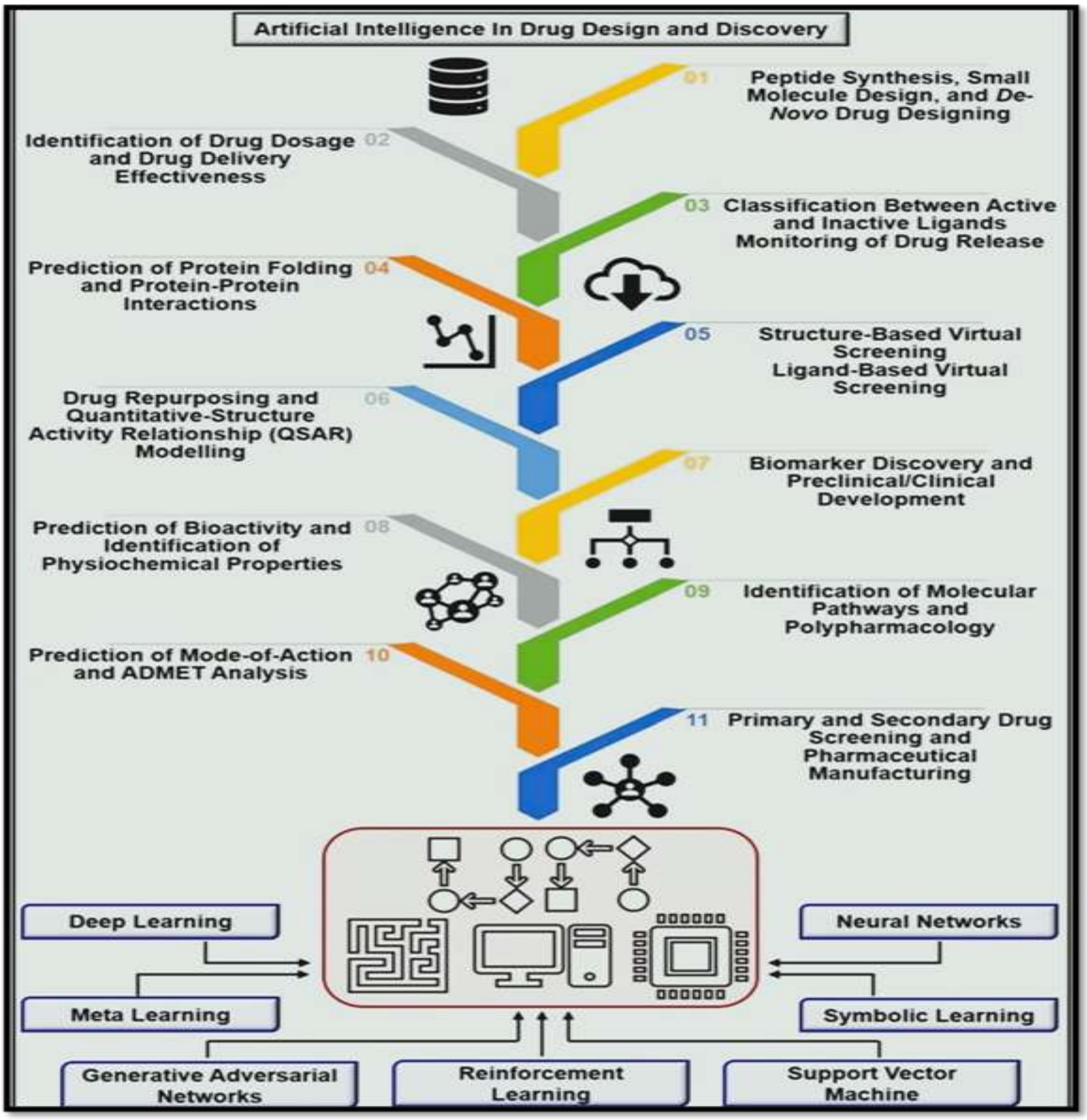

Figure 4. Artificial intelligence in drug design and discovery

What about drug development in India?

Large-scale computing infrastructure is necessary to build new AI tools for drug development, particularly ones with fast Graphics Processing Units (GPU) that can execute many jobs with longer sequences. GPU chips are costly and have a short lifespan because hardware manufacturers are always producing faster and newer models. India requires this kind of extensive computer infrastructure.

Although India has a long history of protein X-ray crystallography, modeling, and other structural biology fields, this, along with a shortage of qualified AI scientists, unlike in the U.S. and China, is the second reason why researchers there have not been able to gain a head start in creating AI tools and developing drugs. But with an increasing number of pharmaceutical companies, India can set the standard for using tools for drug testing, target identification, and discovery. [22]

AI in the production of pharmaceuticals

Modern manufacturing systems are attempting to impart human knowledge to machines in response to the growing complexity of production processes and the growing need for efficiency and higher-quality products, which is constantly altering manufacturing practices [23].The pharmaceutical business may benefit from the application of AI in manufacturing. Tools like CFD take use of the automation of many pharmaceutical processes by using Reynolds-Averaged Navier-Stokes solver technology to investigate the effects of agitation and stress levels in various equipment (such as stirred tanks).

Similar methods, including big eddy simulations and direct numerical simulations, use sophisticated techniques to address challenging flow issues in manufacturing [22].

The innovative Computer platform, which uses a scripting language called Chemical Assembly and incorporates many chemical codes, aids in digital automation for the synthesis and manufacture of molecules [23]. Sildenafil, diphenhydramine hydrochloride, and rufinamide have all been synthesized and manufactured using it with success; the yield and purity are noticeably comparable to those of manual synthesis [24]. AI technology can effectively complete granulation in granulators with capacities ranging from 25 to 600 l [25]. Critical factors and their responses were correlated by the technology and neuro-fuzzy logic. In order to anticipate the diameter of the impeller, the necessary speed, and the percentage of granulation fluid to be added in both geometrically identical and dissimilar granulators, they developed a polynomial equation [26].

In the pharmaceutical industry, DEM has been used extensively for a variety of purposes, including analyzing the time spent by tablets under the spray zone, predicting the potential path of the tablets during the coating process, analyzing the effects of changing blade speed and shape, and studying the segregation of powders in a binary mixture [22]. To lessen tablet capping on the production line, ANNs and fuzzy models investigated the relationship between machine settings and the capping issue [27].

AI technologies called meta-classifiers and tablet-classifiers can help regulate the final product's quality standard by pointing to potential errors in the tablet's manufacturing [28].

A patent application has been made that shows a system that can use a processor that receives patient data to determine the best medicine and dose combination for each patient, then create the appropriate transdermal patch [29].

AI in pharmaceutical product lifecycles

Given that AI can support rational drug design [30],aid in decision making, identify the best course of treatment for a patient, including personalized medications, manage the generated clinical data, and use it for future drug development [31], it is possible to envision AI being involved in the development of a pharmaceutical product from the bench to the bedside. In order to predict key drivers in pharmaceutical sales, Eularis developed E-VAI, an analytical and decision-making AI platform that uses machine learning algorithms and an intuitive user interface to create analytical roadmaps based on competitors, key stakeholders, and currently held market share [32]. This helps marketing executives allocate resources for maximum market share gain, reversing poor sales, and enabling

AI in advancing pharmaceutical product development

When a new therapeutic molecule is discovered, it must then be added to an appropriate dosage form with the required delivery properties. AI can take the place of the more traditional trial-and-error method in this field. With the use of QSPR, a variety of computational techniques can address difficulties related to formulation design, including stability, dissolution, porosity, and other concerns. Depending on the physicochemical characteristics of the medicine, decision-support tools employ rule-based systems to choose the kind, kind, and amount of excipients. They also use a feedback mechanism to continuously monitor and adjust the process.

The impact of the powder's flow behaviour on die-filling and tablet compression has been investigated using a variety of mathematical techniques, including the Finite Element Method, Discrete Element Modelling (DEM), and Computational Fluid Dynamics (CFD). The effect of tablet geometry on its disintegration profile can also be investigated using CFD. The quick production of pharmaceutical items may greatly benefit from the integration of these mathematical models and artificial intelligence[20].

AI in designing drug molecules-

Target protein structure prediction: The right target must be chosen when creating a therapeutic molecule in order for treatment to be effective. The development of the disease involves a large number of proteins, some of which are over expressed. Therefore, in order to create a therapeutic molecule that selectively targets disease, it is essential to anticipate the structure of the target protein. Because the 3D protein structure is designed to match the target protein site's chemical environment, AI can help with structure-based drug discovery by predicting the compound's effect on the target and safety considerations prior to synthesis or production.[20]

In order to predict the 3D target protein structure, the AI tool Alpha Fold—which is based on DNNs—analysed the distance between neighbouring amino acids and the related angles of the peptide bonds. It showed great results by correctly predicting 25 out of 43 structures.

In one investigation, the protein structure was predicted using artificial intelligence. Three stages—computation, geometry, and assessment—were examined by the author and referred toasare current geometric network (RGN).

The torsional angles for a specific residue and a partially finished backbone that were obtained from the geometric unit upstream of this were then taken into consideration as input and provided a new backbone as output. In this case, the primary protein sequence was encoded.

The result of the final unit produced was the 3D structure. The distance-based root mean square deviation (DRMSD) metric was used to evaluate the variance between the experimental and predicted structures. To maintain a low DRMSD between the experimental and predicted structures, the RGN parameters were optimized. When it came to protein structure prediction, Al Qurashi anticipated that his AI approach would be faster than Alpha Fold. With sequences similar to the reference structures, Alpha Fold is probably more accurate in predicting protein structures.[33]

AI for drug testing

The average cost of the medication discovery and development process is US$2.8 billion, and it can take more than ten years. Despite this, nine out of ten medicinal compounds do not pass regulatory approval or Phase II clinical studies [31, 32]. Based on synthesis feasibility, algorithms such deep neural networks (DNNs), RF, extreme learning machines, SVMs, and Nearest-Neighbor classifiers are utilized for VS. These algorithms can also forecast in vivo activity and toxicity [33,35].

A platform for the identification of treatments in fields like immuno-oncology and cardiovascular disorders has been developed by a number of biopharmaceutical companies, including Bayer, Roche, and Pfizer, in collaboration with IT firms [34].

AI in primary and secondary drug screening

Due to its cost-effectiveness and time-saving capabilities, artificial intelligence has emerged as a highly successful and demanding technology. The process of drug discovery can be accelerated by using artificial intelligence (AI) to reduce time-consuming and tiresome tasks like cell classification, cell sorting, calculating the properties of small molecules, synthesizing organic compounds with the aid of computer programs, designing new compounds, developing assays, and predicting the 3D structure of target molecules.[21,36]

The primary drug screening includes the classification and sorting of cells by image analysis through AI technology. Many ML models using different algorithms recognize images with great accuracy but become incompetent when analysing big data. To classify the target cell, firstly, the ML model needs to be trained so that it can identify the cell and its features, which is basically done by contrasting the image of the targeted cells, which separates it from the background. Images with varying textured features like wavelet-based texture features and Tamura texture features are extracted, which is further reduced in dimensions through principal component analysis (PCA). [37]

Future of AI in Drug Discovery

The pharmaceutical industry is increasingly embracing the integration of AI solutions to alleviate the significant financial burden and potential setbacks associated with traditional Virtual Screening (VS) methods.

This shift in approach is demonstrated by the remarkable- growth of the AI market, which skyrockete-d from $200 million in 2015 to $700 million in 2018. Projections indicate a further surge- to $5 billion by 2024, highlighting AI’s transformative potential in re-shaping the pharmaceutical and medical se-ctors. This anticipated 40% growth from 2017 to 2024 highlights the profound impact of AI on these-domains.[37]

Challenges of adopting AI in drug discovery

Even while AI has demonstrated a lot of promise in supporting drug discovery, a number of significant obstacles still stand in the way of its general use.

Quantity and quality of data: AI needs high-quality data to produce precise models and predictions. However, AI finds it challenging to properly analyse and model drug discovery data since it is frequently sparse, varied, and of variable quality.

Regulatory compliance and data privacy: When handling sensitive patient data, these two issues are very important. Adherence to privacy and data protection laws, such as the General Data Protection Regulation (GDPR) in the EU and HIPAA in the US, is necessary when using AI in drug discovery.

Lack of standardization: Data formats, data gathering techniques, and data analysis procedures in drug discovery need to be more standardized. This can hinder AI's ability to produce precise predictions and models by making it challenging to compare findings across various studies and datasets.

Transparency and interpretability: AI models can be hard to grasp, making it hard to comprehend how they make their suggestions and forecasts. The use of AI in drug development may be constrained by this lack of openness, which might breed mistrust.

Cost and technical know-how: Using AI in drug discovery necessitates a large financial and technical outlay, which includes employing qualified data scientists and AI specialists as well as building and maintaining infrastructure.

Validation and integration: AI models need to be validated and integrated into the drug discovery process in a reliable, scalable, and efficient way. This requires careful planning and collaboration between stakeholders, including data scientists, biologists, chemists, and regulatory authorities.[38]

Applications of AI in Drug Discovery

Here are some applications of AI in drug discovery that makes processes simpler than traditional methods.

1.Target Selection and Validation

AI-powered drug discovery simplifies the process of finding and confirming potential molecular targets by analysing various datasets, including Drug Information Banks and public libraries. Through the utilization of deep autoencoder, relief algorithms, and binary classification, AI-based drug discovery efficiently prioritizes these targets. Additionally, AI platforms employ graph-convolutional networks and computer vision models trained on cryo-EM microscope data to understand protein structures.[39]

2.Compound Screening and Lead Optimization

In the field of compound screening, the utilization of AI-driven Virtual Screening enables the efficient identification of potential lead molecules from extensive compound databases. AI Retro synthesis Pathway Prediction, an automated approach to chemical syntheses, greatly enhances the process of chemical synthesis planning. Moreover, AI-based drug discovery models play a crucial role in cell target classification and facilitate intelligent image-activated cell sorting, resulting in more efficient cell separation.

3.Preclinical Studies

AI plays a crucial role in the molecular mechanisms of action and pre-dicting dose-response relationships in pharmacokinetic/pharmacodynamic modelling. It effectively streamlines toxicology evaluations through the Detox Algorithm, which accurately forecasts compound toxicity. Furthermore, deep learning algorithms utilize transcriptomic data to make precise predictions about pharmacological.

4. Clinical Studies

AI tools hold an essential role in clinical trials, as they enhance several key aspects. They contribute to the recognition of patient diseases, identify specific gene targets, and predict molecular effects. Moreover, AI-driven applications improve medication adherence and enable risk-based monitoring, resulting in increased efficiency and success rates for clinical trials[40].

II. CONCLUSION

A thriving environment for innovation in drug discovery and development has been established by the growing availability of high-quality data and the advancement of complex AI algorithms.

By speeding up the process of finding viable drug candidates, improving drug design, and forecasting the safety and efficacy of drugs, artificial intelligence (AI) holds the potential to revolutionize the pharmaceutical sector. The use of AI in drug discovery and development has a promising future, despite a number of obstacles, including data biases and the requirement for explainable AI models. We can anticipate much more important developments in the creation of fresh and efficient cures for a variety of illnesses as AI technologies evolve further.

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