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Artificial Intelligence-A Key Note Biomarker in Drug Discovery and Development

Running Title: ARTIFICIAL INTELLIGENCE

Madhavi Nimmathota[a*], Merlin T Babu[b], S Tanusri[c], N Aishwarya[d], Rama Rao T[e]

[a,,b,c,d] *CMR College of Pharmacy, Affiliated to JNTUH, Medchal, Kandlakoya, Hyderabad-500090, India*
[e] *Professor and Principal, CMR College of Pharmacy, Affiliated to JNTUH, Medchal, Kandlakoya, Hyderabad-500090, India*
[a*] *Email: madhavi@cmrcp.ac.in*

Abstract

The application of artificial intelligence (AI) has recently accelerated in several societal domains, with the pharmaceutical sector leading the way. This paper highlights the useful applications of AI in the pharmaceutical industry, including medication discovery and development, drug repurposing, and pharmaceutical quality improvement. Among others, productivity, clinical trials, etc., have reduced the workload of people and expedited the completion of goals. Crosstalk about the methods and instruments used to enforce AI, ongoing problems, and solutions to them is also explored, as is the role of AI in terms of efficiency, accuracy, and speed. AI has the potential to revolutionize the drug discovery process. However, the availability of high-quality data, addressing ethical issues, and using AI effectively all depend on an understanding of the limitations of AI-based techniques. This article discusses the advantages of AI in this field, along with potential solutions. The suggested barriers to the situation are the addition of data, comprehensible AI, and the incorporation of the potential benefits of AI in the pharmaceutical industry, as well as how it compares to conventional experimental methods. This paper underlines the potential of artificial intelligence in drug discovery and gives details about the possibilities for attaining.

Keywords: Potential; Machine; Discovery; Artificial intelligence**.**

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* Corresponding author.

1. Introduction

In ancient days, there were no smart devices to provide much information about the updated technologies. When the time passed, many were introduced to web-based systems. Watson, a scientist, has developed AIadvances for people in a triangle manner. In the field of medicine and pharmaceuticals, changes may benefit life. These fields focus mainly on creating and discovering new chemical compounds and mixtures, which are the solutions to physical and psychological suffering. For many years, the regulatory system controlled the manufacturing of the products, which safeguarded the quality of the final drug product by testing the raw materials, process materials, end product characteristic features, batch-based operations, and fixed process conditions. The drug and biopharmaceutical industries lack the source of novel technologies, which led to a deficiency in the development of new principles and definitions in chemical and mechanical engineering [1].Discovering and manufacturing complex processed medicines for safe human use on a commercial scale. Current developments in genomics and diagnostics have enabled novel and innovative pharmaceutical products and approaches depending on new analytic instruments and precise portions. Medicines that are adjusted to the patient's biology would increase the efficiency of this industry. AI is being used more frequently, which may probably alter the clinical evaluation and training that were conducted earlier. To ensure the potential of AI to improve medical care, doctors can collaborate in the development of this technology for application in the medical and pharmaceutical industries. Currently, AI uses primarily four different methods in the pharmaceutical sector. The initial step is the evaluation of illness severity and the forecasting of whether, before starting the treatment, Second, it is employed to avoid or address difficulties as a part of treatment. Its third primary usage is as a patient-assistance technology during medical procedures or operations. Last, but not least, it is utilized to ascertain the rationales behind the usage of specific tools or substances during therapy and to create or extrapolate new uses for tools or substances to increase safety and efficacy [2].

1.1. Classification of AI

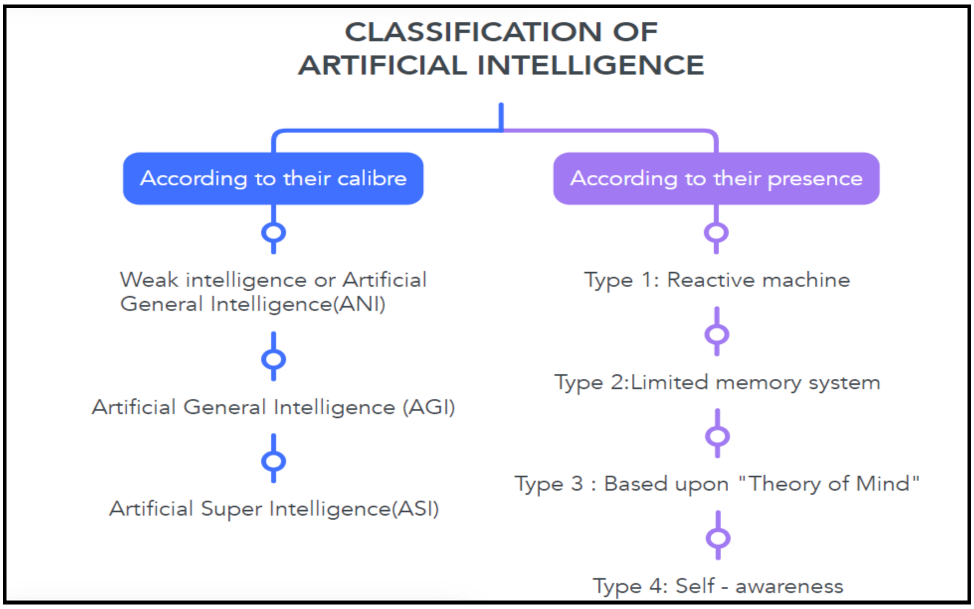

Figure 1: Types of AI based on its calibre and presence

Additionally, AI plays a more general role in administering and examining huge amounts of data. A modern paradigm known as "big data" describes the collection of very massive datasets and their coupling with advanced analytics to produce new knowledge or insights from these databases. Thus, as data volumes grow, conventional data storage techniques in the pharmaceutical business are rendered outdated [2]. As a result of data mining in this business, big data presents a significant possibility for more in-depth study and can improve pharmaceutical manufacture by adopting a three-step data management method after collection that involves the following steps: extraction and packaging of large amounts of heterogeneous and dispersed data, uniform data configuration formatting, utilising multiple analytical tools, and data analysis to produce a product, whose interpretation may be used to guide decisions on what substances or medications to create or methods to employ to increase productivity .

The detection of molecular entity traits against those of known compounds is accomplished via passive AI. The exactness of the medication delivery methods chosen by AI is crucial for effective therapy [2]. AIin medicinal chemistry has attracted a lot of interest recently as a potential way of transforming the pharmaceutical business. Drug discovery, the process of finding and creating novel drugs, is a difficult and time-consuming task that has historically relied on labour-intensive methods like high-throughput screening and trial-and-error research. However, there are obstacles and restrictions in the application of AI to the creation of novel bioactive chemicals. Further study is required to properly understand this issue, and ethical issues must take into account the benefits and restrictions of AI in this field. Despite these difficulties, it is anticipated that AI will greatly contribute to the creation of novel treatments and pharmaceuticals in the coming years [9,10].

Recent developments in AI might assist in reversing this trend and enhancing pharmaceutical research and development. Early deep-learning presentations to the pharmaceutical business in 2014 and 2015 were met with scepticism and were abandoned. Many pharmaceutical firms began collaborating with AI start-ups and academia in 2017 or launched internal research and development initiatives. The method of deep learning spread quickly into many fields of biomedical research, from training (DNNs) on transcriptional response data to predict the pharmacological effects of small compounds (1) and the production of biomarkers (2) to the generation of new chemistry. A special edition of Molecular Pharmaceutics titled "Deep Learning for Drug Discovery and Biomarker Development" will examine how AI is being applied in chemistry and biomedicine [1]. Modern machine learning methods might clarify some of the models and deepen our understanding of biology and chemistry. The only true indicator of success in using artificial intelligence for drug development is the positive testing of AI-generated compounds for the identified targets, even if research in this area is rapid. Clinical experiments utilising AI have yet to be proven. AI is being used to compete for human validation and effective treatments.

1.2. How AI is Being Used

Pre-clinical phases of conventional drug discovery are notoriously lengthy and expensive, spanning three to six years on average, but a variety of AI technologies are revolutionizing almost every stage of the drug discovery process, holding great promise for changing the industry’s pace and cost. Physicochemical properties When forecasting to developmentof a new medicine, physicochemical characteristics, including solubility, partition coefficient (log P), degree of ionisation, and intrinsic permeability of the drug must be taken into account because they have an indirect impact on its pharmacokinetics and target receptor family [3].

1.3. Analysis of Bioactivity

The affinity of drug molecules for the target protein or receptor determines how effective they are. The therapeutic effect cannot be produced by drug molecules that do not interact with or have an affinity for the targeted protein. It’s also feasible, in some circumstances, which therapeutic compounds interact with toxicity caused by unwanted proteins or receptors. As a result, it is essential to forecast drug-target interactions using drug target binding affinity (DTBA). AI-based approaches can estimate a drug’s binding affinity to determine the feature vectors, feature-based interactions to identify the chemical moieties of the medication and the target [3].

1.4. Toxicity Prediction

To prevent hazardous effects, it is essential to forecast the toxicity of every therapeutic molecule. The cost of developing new drugs is increased by the frequent use of cell-based in vitro assays as preliminary investigations, followed by animal trials to determine a compound’s toxicity. Online instruments, including LimTox, pkCSM, admetSAR and Toxtree[3].

2. AI in the Field of Pharmacy

- It is one of the top technologies which shape the future of pharmacy.

- Pharma industries have been developing for cure and treatment since long back. Traditionally, the design and manufacturing of drugs required several years, length clinical trials and huge costs, with the rise of 21st century technologies, this has been changing.
- In future we will see completely different drug designs, manufacture and clinical trials.

2.1. Importance of AI in Pharmaceutical Industry

- Pharmaceutical industry can accelerate innovation by using technological advancement.
- The recent technological advancement that comes to mind would be artificial advancement that comes to mind be artificial advancement such as visual perception, speech recognition, decision-making and translation between languages.
- An estimate by IBM shows that the entire healthcare domain has approximately 161 Billion GB of data as of 2011.
- With humongous data available in the domain, AI can be of real help in analyzing the data and presenting results that would help in decision making, saving human effort, time, money and thus help save lives.

2.2. Future Aspects of AI

- AI is able to design new drugs
- Find a new drug combination.
- Deliver clinical trials within minutes.
- Drugs are not tested on real humans and animals, but on virtual model that are Engineered to mimic the physiology of organs.
- Robots help in the manufacturing of medication as well as their distribution
- Counterfeiting drugs become almost impossible.
- Block-chain technology secures the entire distribution channel.
- Local pharmacist's 3D prints personalized drugs in any shape and desired dosage.

Companies in today's data-driven society never miss a chance to seize a market opportunity to improve, automate, and streamline company processes. This rising wave is fueled by data science. Thanks to artificial intelligence, businesses may now analyze data at the highest level of efficiency, having a significant impact on their overall operations.The use of AI by various businesses will lead to impressive growth in the upcoming years. According to research, the global AI market would generate $89.8 billion in annual revenue by 2025. In this situation, the pharmaceutical sector is hardly an exception. Artificial intelligence has unquestionably had an impact on the pharmaceutical sector. Around the world, many pharmaceutical companies have already begun to use AI in their operations. The pharmaceutical business has benefited from the development of this cutting-edge technology, which has a bright future.

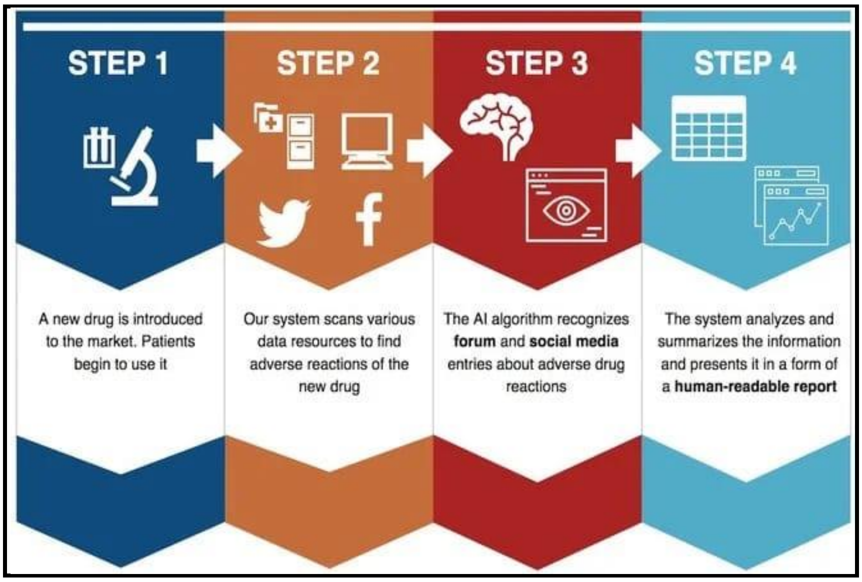

Figure 2: Steps involved in drug discovery

2.3. Situation Today in the Pharmaceutical Industry

AI, broadly speaking, is the use of computer systems to carry out tasks that typically require human intelligence.

It can be incredibly helpful in managing data, providing findings that encourage better decision-making, and saving time, money, and human effort. However, many businesses who run their healthcare operations using conventional ways have not yet embraced this technology. But what they fail to realize is that the pharmaceutical sector can be impacted in a number of different ways without the use of artificial intelligence:

1. The gathering and processing of medical data may be slowed down.
2. Lack of data and medical records availability
3. Expensive and drawn-out medicine research and development procedure

Therefore, the use of AI and machine learning is crucial for making all procedures related to healthcare efficient, affordable, and smooth.

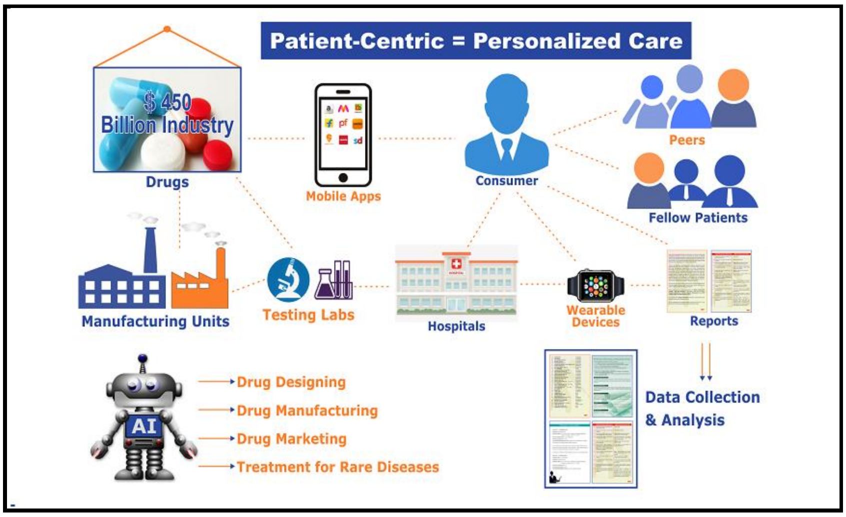

Figure 3: AI in the line of pharmaceutical industry

3. Machine Learning Applications in the Pharmaceutical Sector

Machine learning, which is a component of AI, enables an algorithm or computer program to learn a task and execute it without explicit programming instructions. It places a lot of emphasis on creating computer programs that can access data and use it to learn on their own. The system can operate on its own if everything is thoroughly inspected and the code is applied correctly. The use of machine learning in the pharmaceutical business has improved the effectiveness and seamlessness of the clinical and healthcare process. It has created new opportunities in this sector. The top six uses of machine learning are shown below [4,5].

1. A Better Diagnosis Procedure

Doctors may readily access vast volumes of patient data by using machine learning in the pharmaceutical sector, improving diagnosis and treatment. This technology is being used by renowned medical facilities all over the world to keep electronic medical records [4]. The records are used by doctors to comprehend how a patient's health may be affected by specific genetic characteristics or how a new medicine may benefit that patient. They may also have a thorough understanding of the illnesses and recommend the best course of action. These digital health records reduce costs and save time.

2. Clinical Trial Research Advances

Clinical trial research is no longer a dangerous task for developing new medications. Healthcare businesses can use machine learning to extract pertinent EMR data and read through physician notes. The information gathered can then be used to identify the best patients for the trial operation. Predicting patient churn is achievable at any time during the operation. Through smart phones and other wearable tech, people may easily send relevant information. In this way, gathering important data from patients has become quick and simple. Even patients can now easily share their data for clinical trial processes with just one click. Additionally, the data is highly accurate, relevant, and of outstanding quality.

3. New Approaches to Drug Discovery

Several steps of the drug development process are improved by machine learning:

- Machine learning offers enormous potential for use in the early stages of drug discovery, including preliminary screening of medicinal compounds and success rate prediction based on biological factors.
- Machine learning makes it simple to find new patterns in the information generated during the generation of diverse biomedical datasets. In short, machine learning may analyze any type of data and then be used to develop creative approaches to the discovery of new medicines.

4. Improved Patient Care

The challenge of tracking patient data and monitoring it while making judgments in real time has long since vanished. Machine learning has made it simpler than ever to manage vast volumes of data and identify potential remedies for various illnesses. Using data from a patient’s test results, charts, and metrics, the system forecasts in real-time and makes therapy suggestions for critical care. In other words, machine learning makes it possible to estimate effective therapies using information from medical records, improving healthcare.

5. Innovation in Drug Research and Development

Reputable pharmaceutical companies throughout the globe are using machine learning to speed up the discovery of new medicines. The complex biological networks can be resolved by machines with a high level of pattern recognition ability. In turn, this can advise pharmaceutical companies to steer clear of drugs with a high risk of failure while assisting in the identification of medications that may function in specific patient populations.

6. Improved Epidemic Prediction Accuracy

Based on data gathered from the internet, social media, satellites, and other well-known sources, machine learning technology is also being used to track and predict epidemic outbreaks around the world. For instance, research shows that the "Malaria Outbreak Prediction Model using Machine Learning" serves as an early warning tool to forecast potential malaria outbreaks, raise awareness among the public, and inspire healthcare professionals to make better decisions more quickly. This machine learning application is helpful, especially for those nations that frequently lack enough medical infrastructure, sufficient understanding of ailments, and simple access to the best treatments [6].

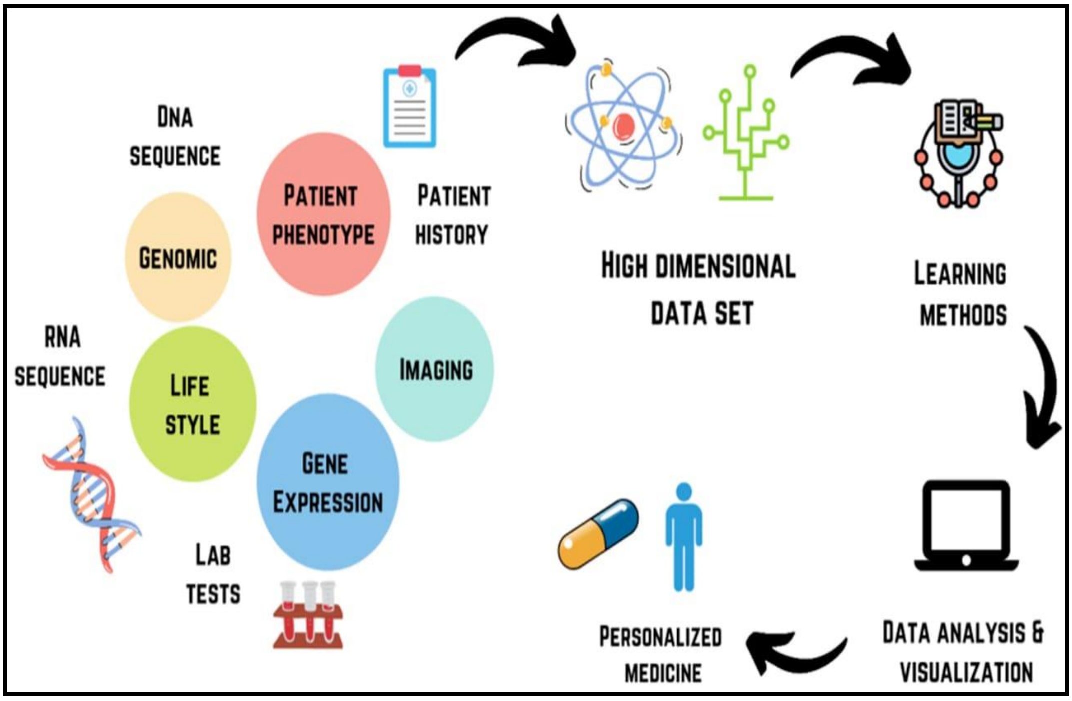

Figure 4: Various applications in machine learning

4. Applications of AI in Pharmaceutical Industry and in Hospital Pharmacy

AI is used in a variety of ways in hospital pharmacy-based health care systems, including organizing dose forms for specific patients and choosing the best or most available treatment plans or administration methods [7,9]. Those are stated as:

I) Keeping Track of Medical Records

Keeping track of patient medical records is difficult work. The gathering, storing, normalizing, and tracking of data are made simple by putting the AI system in place. The Google Deep Mind Health Project, a Google creation, aids in quickly digging up medical records. Consequently, this project is beneficial for improved and quicker medical attention.

Ii) Designing Treatment Plans

AI technology makes it feasible to create effective treatment programmers. The AI system is required to maintain control when a patient's health gets severe and choosing an appropriate treatment plan becomes challenging. The treatment plan provided by this technology takes into account all of the prior data and reports, clinical knowledge, etc.

III) Assisting in Repetitive Work

AI technology also helps with some monotonous duties, such as studying X-ray images, radiology reports, ECHO, ECG, etc., to find and identify illnesses or abnormalities [5]. IBM's Medical Sieve algorithm is a "cognitive assistant" with strong analytical and deductive skills. To enhance patient conditions using deep learning and medical data, a medical start-up is required. For each bodily component, there is a specialized computer programmer that is employed in particular illness situations. For practically all imaging analysis types, including X-ray, CT scan, ECHO, ECG, etc., deep learning may be used.

IV) Health Support and Medication Help

In recent years, the usage of AI technology has been found to be effective for both medication assistance and health support services. The voice and visage that Molly (a virtual nurse created by a start-up) hears are kind. Its purpose is to support patients with chronic conditions in between medical appointments and to assist individuals in directing their own care. The smart phone camera software Ai Cure keeps track of patients and helps them manage their diseases.

V) AI Aids Individuals in the Healthcare System

It has the ability to compile and contrast data from social awareness algorithms. The extensive data stored in the healthcare system includes a patient's medical history, treatment history profile going back to their birth, habits, and way of life.

5. Approaches for Drug Discovery

The drug discovery process starts with the findings that have been obtained from many resources, including high-throughput screening models, fragment screening models, computational models, and reported existing data. An illustration of the drug discovery process Computer-assisted design methodologies may be used in the drug discovery process to analyze the structural characterization of drug molecules either directly or indirectly before organic drug molecule synthesis is carried out. The drug molecules that have been created or the drug compounds that have been gathered are placed through high-throughput screening in the first assay, and after that, they are counter-screened and assessed for their bioavailability in secondary assays along with successful structure-activity relationship (SAR) analysis.

Drug discovery techniques alternate between induction and deduction. As a result, obtaining the optimized lead molecules is eventually guided by the interchangeable cycle of inductive and deductive reasoning. The automation of some steps in the inductive-deductive cycle reduces uncertainty and inaccuracy, increasing the efficiency of the drug development process. By using deep learning software, such as "NVIDIA DGX-1," chemical and pharmaceutical producers may study and derive information from various patents as well as genetic data-based scientific research. Humans are unable to use all of the knowledge available to enhance scientific research. Supercomputers with AI are able to gather and evaluate data in order to identify associations between substances and provide innovative medication molecules. The use of chemical space is an issue for AI applications in the drug development process. Since the required molecules may be computationally iterated, the chemical space really provides the stage for the identification of novel compounds. Additionally, the discovery of target-specific, efficient compounds is aided by machine learning and associated prediction techniques. The hardest aspect of the whole phenomenon is choosing a successful new medication molecule from a huge number of pharmacologically active chemical entities.

Fewer molecules are processed with significantly more confidence in their activity, to benevolent AI. De novo design in this context necessitates a grasp of organic chemistry for the synthesis of in silico compounds and the virtual screening models that serve as substitutes for numerous biochemical and biological tests to determine the efficacy and toxicity profiles. De novo design is an approach to drug development that aims to create newer active compounds without the use of reference molecules. Finally, active learning algorithms enable the identification of novel compounds with potential anti-targeting effects for illnesses or disorders. Along with the readily available data on the small molecule modulator probes or the characteristics of structural biology, a variety of in silico methods for the selection of profiles, such as ligand-based design approaches or molecular structure-based design approaches, may be used. The next generation of AI is being developed for molecules in silico. There are several software options and suggestions available for it. This design is not helpful for the development of new drugs, but it is related to the creation of components that are difficult to synthesize1. Although recursive neural networks are used in de novo design, they were first developed for the purpose of analyzing natural language. Recursive neural networks accept sequential data as input.

The field of artificial intelligence has an intriguing technique known as "Variational Auto encoder" that uses two neural networks: (i) encoder networks and (ii) decoder networks. Encoder networks and decoder networks, respectively, translate vectors from the latent space into the chemical structures using a real-value continuous vector as the latent space and vice versa. The authors call for the latent extent description in order to train a model that depends on the synthetic accessibility score (SAS) and QED drug-likeness score.Then, a passage of molecules with improved target qualities can be obtained. The performance of a "variational autoencoder" and an "adversarial autoencoder" was compared. Compared to the "Variational Auto encoder," the "Adversarial Auto encoder" has a larger capacity for constructing significantly more genuine molecular structures throughout their creation mode.

Drug compounds can be designed using generative adversarial networks (GANs). The technique can create images that are photorealistic from text representations. Kadurin and his colleagues. (2017) used GAN in a study to suggest drugs with anticancer properties. This technology also allows for the production of new data based on imagination or genuine data. Learning from massive data sets is not necessary for the development of future AI. The formerly difficult-to-solve problems can all be handled by the new AI technology. This innovative technology aids scientists and researchers in the identification and selection of potential chemical agents based on their efficacy, safety, and patient selection for clinical trials1. As a result, AI is valuable in medication delivery since it may prioritize molecules based on how easy they are to synthesize or design practical tools that have been shown to be effective for the most advantageous synthesizing approach.

6. Approach for Drug Delivery System

Designing drug delivery systems typically comes with some drawbacks, such as the inability to foresee the link between formulation parameters and reactions. This is connected to both the treatment results and the unexpected events. On-demand dosage modification, drug release rates, targeted release, and drug stability are crucial considerations when constructing various types of intelligent drug-releasing systems. The appropriate algorithms are helpful for managing the quantity as well as the duration of drug release in self-monitoring systems for medications. As a result, AI techniques are helpful for predicting the effectiveness of medication dosing and the potential for drug delivery.

AI usage spread to different dosage forms; those are sequentially mentioned as follows:

SOLID DISPERSION: Poloxamer 188 and Soluplus® were used to create solid carbamazepine dispersions utilizing ANN modeling together with experimental design. To increase the solubility and rate of dissolution of carbamazepine, solid carbamazepine dispersions were prepared. These solid dispersions of carbamazepine-Soluplus®-poloxamer 188 were created using the solvent casting method. In a study, an ANN model with the logistic sigmoid activation function has already been used to examine the relationships between various factors and the characteristics of drug dissolution in order to maximize the drug dissolution rate.

EMULSIONS AND MICROEMULSIONS: ANNs have also been used to generate stable oil-in-water emulsion formulations. In this paper, the optimization of the fatty alcohol content to create oil/water emulsions was examined. The concentrations of lauryl alcohol and time were the unstable variables (factors) studied in this paper. The reliable variables (responses) were conductance, viscosity, zeta potential, and droplet size. Based on validation testing, it was discovered that ANN-predicted values had a strong connection to the experiment's results. ANNs have also been used in the formulation design of microemulsions, where it was simple to anticipate accuracy based on the nature of the microemulsion from the formula. The formulation of stable microemulsions containing anti-tubercular medications like rifampicin and isoniazid for oral administrations has previously been predicted using ANN modelling. Data from the pseudo-ternary phase triangle diagrams displaying the oil constituents and surfactant combination were utilized for the ANN modeling’s testing and validation.

TABLETS: Static and dynamic ANNs have been used in the design of matrix tablets to model the dissolving profiles of various matrix tablets. Monte Carlo simulations and a genetic algorithm optimizer tool were used in this study to simulate these systems using the ANN method. Elman dynamic neural networks and decision trees were employed by the researcher to accurately forecast the dissolving characteristics of hydrophilic and lipid-based matrix tablets with regulated medication release patterns. The Elman neural network-based modeling revealed the effective modelling of drug-releasing patterns by various formulas of hydrophilic as well as lipid-based matrix tablets, in contrast to the majority of frequently used multilayer perceptron and static networks. In a study, multilayer perceptron with feed-forward back propagation technology was used to manufacture matrix tablets for prolonged release of the anti-diabetic medication metformin HCl. To create the optimized formulations, the matrix tablets' *in vitro* metformin HCl release pattern was optimized. In a different study, ANNs were used to improve the formulation of nimodipine matrix tablets for controlled release. The formulation design of glipizide-releasing osmotic pump tablets uses a combination of statistical optimization and ANN-based modeling. These glipizide-releasing osmotic pump tablets were tested for dissolving, and the various formulation and process factors were also optimized and examined using ANNs.

7. Conclusion

Over the past few years, there has been a noticeable increase in interest in the applications of AI technology. Found for reading and assessing some crucial pharmacy disciplines, including medication discovery and dosing. Humans create knowledge and solve issues and making decisions. Applications for automated work flow and databases for the use of AI in successful analysis. Techniques have proven to be effective. In light of the application of AI techniques, the creation of new methods, predictions, and evaluations of numerous theories associated factors are simply accomplished thanks to the capability of cost-effectiveness and fewer hours spent.The growth in the number of start-ups in this industry may be due to the continued development of AI and its impressive tools, which attempt to lessen the difficulties experienced by pharmaceutical businesses in both the medication development process and the full lifespan of the product.

8.Abbreviations

DNNs - Deep Neural Networks,DTBA -Drug Target Binding Affinity,

QED - Quantitative Estimate of Drug, ANN- Artificial Neural Networks, GAN-generative adversarial network

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