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Review

A Boom of Artificial Intelligence In Pharmaceutical Industry- A Review

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Abstract

Artificial intelligence (AI) is a promising and specialized field in computer science that utilizes machines and mathematical algorithms to efficiency process, analyze and predict the data. The research in AI has great potential in pharmaceutical and healthcare system including drug discovery, drug repurposing, determining pharmacodynamics and pharmacokinetic parameters, drug dosage form designing and disease diagnosis. Artificial intelligence has transformed the way biotechnology and pharmaceutical technology performs with the help of pharmacists (researchers and scientist) to a great extent. Artificial intelligence plays a crucial role in pharmaceutical sector as it decreases the human intervention, facilitates the R&D pharmaceutical process, equipments required for curing the disease and medical illness, pharmaceutical productivity, promote innovation, drug discovery, drug delivery formulations development, poly-pharmacology, hospital pharmacy and clinical trials. The AI technology involves deep learning models and neural networks for research in pharmaceutical sector. AI is known for its cost effective, fast and accurate result predictions with high efficiency and personalization in medicinal sector. This review focuses on the Artificial intelligence, history, application of AI and benefits and limitation in pharmaceutical and healthcare sector.

Keywords: AI, machine learning, drug discovery, drug repurposing, neural networks, Pharmacodynamics and Pharmacokinetics, QSAR

I. INTRODUCTION

Artificial Intelligence is a field of computational technology that has flourished in the past decade in every aspect of Science and technology including pharmaceutical business [1-3]. Artificial intelligence has transformed the way biotechnology and pharmaceutical technology performs with the help of pharmacists (researchers and scientist) to a great extent [4-10]. Artificial intelligence plays a crucial role in pharmaceutical sector as it decreases the human intervention, facilitates the R&D pharmaceutical process, equipments required

for curing the disease and medical illness, pharmaceutical productivity, promote innovation, drug discovery, drug delivery formulations development, poly-pharmacology, hospital pharmacy and clinical trials [11-13].
Artificial intelligence comprise Machine learning, deep learning, neural network models such as recurrent model, artificial neural model, deep neural network model, natural language processing, physical robots and robotic automation [14-18]. All these components have wide applications in pharmaceutical and healthcare sector that includes:

- Data imaging for early diagnosis of disease particularly cancer that leads to rapid prevention of disease
- Comprehending human speech for exploring data from doctor’s notes and laboratory reports
- Rapid Decision making and diagnosis
- Customizing treatment options
- Enhancing patient outcomes
- For nursing and telemedicine such as cleaning, radiology and surgeries
- Drug discovery and production such as generating QSAR for drug screening, facilitating data processing in drug development, and quality control [19]
- Choosing the most appropriate excipient, manufacturing process and ensuring that the specifications are met
- Robotics automation aids in dispensing medicaments, filling prescriptions, supervising or managing supply chains, updating patients records and bills, logistics and marketing [20-24]

History of Artificial Intelligence

The concept of artificial intelligence started back in 1955 by Herbert A Simon and Allen Newel with John McCarthy (known as the Father of Artificial intelligence) and introduced the term Artificial Intelligence worldwide [25]. In 1956, Simon and Newell developed “The Logic Theorist” at the conference organized by Dartmouth College. They categorized Artificial intelligence into 4 types: Reactive machines, Theory of minds, Self awareness, Limited memory [26]. In 1966, Watson observed that artificial intelligence has the capability to understand spoken language. In the same year, Joseph Weizenbaum developed the 1st chatbot which was named as “ELIZA” [27]. In 1972, Japan built the first Intelligent Human Robot called “WABOT-1”. During the 1974-1980 phase, the researchers and computer scientists lacked government funding and struggled for research in Artificial Intelligence. The period of 1980-1987 was known as “A boom in Artificial Intelligence” where a computational program was developed which was able to make decisions just like humans and a National conference on “Artificial Intelligence” was conducted in 1980. Again during the phase of 1987-1993, the graphical pattern of growth in Artificial Intelligence fell down due to withdrawal of funding by government because of high cost of research in AI and slow rate of growth in AI. In the year 1997, IBM Deep Blue known as the first computer to participate in World Chess Champion defeated Gray Kasparov. In 2002, the concept of Artificial Intelligence was used in designing vacuum cleaner and an advanced Vacuum Cleaner was designed named “Roomba”. In the year 2006, the concept of Artificial Intelligence was used by big business MNCs and social media websites such as Netflix, Facebook and Twitter. In 2011, the IBM Watson won the game show “Jeopardy” by solving maximum number of riddles. In 2012, Google introduced “Google Now” feature whereby google users can receive predictions with information. In 2014, a chatbot named “Eugene Goostman” won the competition Turning Test. In 2018, an IBM “Project Debater” debated with 2 expert debaters and performed well. In 2022, NASSCOM reported that Artificial intelligence has emerged as powerhouse in IT sector and has became the home for more than 500 AI startups which is almost 33% hike when compared to previous year. It has been projected that the AI market in India can reach to $17billion by 2027 and can grow by 17.94% by 2030. Globally, it is estimated that the growth rate of Artificial Intelligence can increase by 15% by market volume of US$738.80 billion by 2030 [28, 29].

Statistical growth of Artificial Intelligence in Pharmaceutical Industry

In a survey it was found that about 80% of life sciences and pharmaceutical professionals have been using the technique of Artificial Intelligence for Drug discovery.

About 95% of Pharma Industries have invested in Artificial Intelligence for Pharmaceutical growth. AI has helped to accelerate the pharmaceutical drug discovery process from five to six years to directly one year. This can lead to drug development process completion within 4 years and save more than 26 billion US dollar. Moreover, AI has the potential in reducing the time taken in clinical trials by 80% and cost reduction by almost 70%. The acceleration in drug development process has aided a lot in drug discovery process during pandemic (COVID 19).

It has been estimated that AI in pharmaceutical industries has the potential to grow upto 350 to 410 billion US Dollar by financial year 2024-2025. During the period of 2021-2028, AI is estimated to grow annually by 40.1% and 52.7% in the field of cancer diagnosis and genomics respectively.

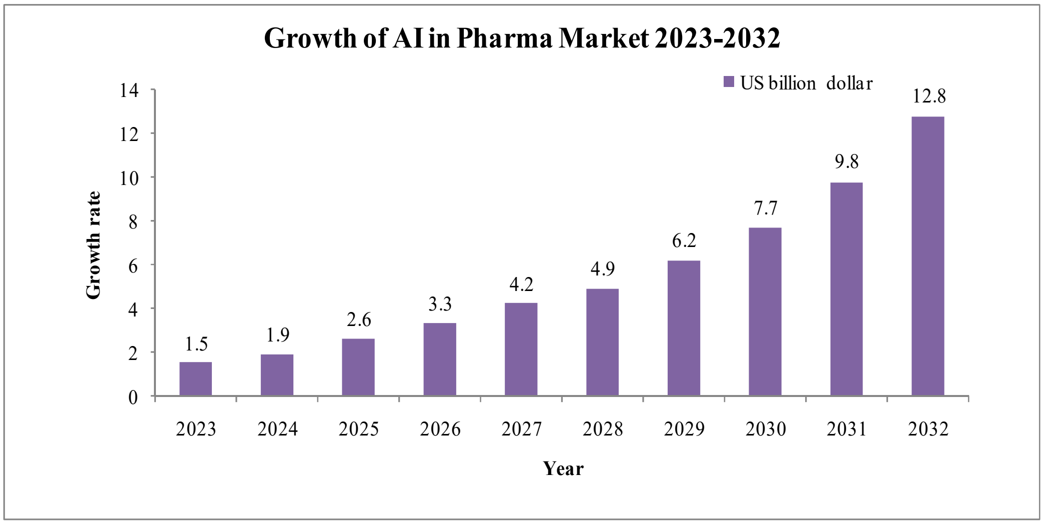

Fig 1: Forecast of growth rate of AI in Global Pharmaceutical market from 2023-2032 (Source: Statista)

Applications of Artificial Intelligence

In Dosage Form Designs

For the efficacy and effectiveness of drug it is necessary to determine the accurate dosage form design. The rate of permeation is determined by route of administration for efficient drug delivery system. The drugs permeate either through active diffusion or passive diffusion process. The active diffusion process involves the direct targeting of the drug at site of action which is monitored by membrane transport and complicated biological interactions whereas the passive diffusion depends on the chemical characteristics of the drug molecules [30]. Hence, to determine the permeation rate or route of administration it is necessary to validate or estimate the pharmacokinetic characteristics of the drug molecules. In order to estimate the pharmacokinetic parameters and to predict the preclinical models a computational model is applied nowadays for pharmaceutical R&D [31, 32].

Artificial intelligence is an advanced technology that is used for analyzing pharmacokinetic data, artificial neural networks and offer databases such as genomes, chemicals and phenotypes for complete understanding of drug molecules interaction [33]. AI is also used to investigate the effect of drug delivery system on the pharmacokinetic properties of the drug and employing knowledge for drug disposition and toxicity. AI tools can further help in determining the drug development, new therapeutic use for older API, decision making and recording vast data of R&D, drug distribution and drug interactions. E-VAI is an analytical tool designed by Eularis utilizes Machine Learning algorithms and user friendly interface that creates an analytical roadmap based on market factors such as stakeholders, competitors and market share [34-36].

For Drug Delivery

Artificial Intelligence, Machine Learning or computational pharmaceutics in the form of multiscale modeling methodologies seeks to improve the drug delivery system, analyze massive set of data and determine drug behavior that aids the pharmaceutical researchers to assess and optimize the drug delivery system without any tedious and manpower consuming hit and trial studies [37]. AI aids in reducing the associated data errors and other adverse events [38]. With the help of AI the pharmaceutical research scientists have gained several advantages such as AI has reduced the time needed for production of drug development, boost productivity and reduced the cost associated in R&D [39, 40].

AI has also helped the scientist in determining the drug-drug interactions and drug-human body interactions, side effects associated that leads to better and personalized treatment options, ensuring patient's safety and reducing adverse events [41]. AI algorithms aids in estimating the complicated drug interactions, predicting physiochemical properties of drug, *in vitro* drug release, drug release kinetics (Zero order, First order, Korsemeyer and Higuchi release kinetic model) and drug stability. AI algorithms are also useful in estimating the *in vivo* pharmacokinetic parameters, drug distribution and *ivivc* research [42, 43].

Artificial intelligence has been very useful in formulation of solid dosage forms such as tablets, granules and capsules [44, 45]. During the formulation of tablets, AI alongwith artificial neural networks and logics aids in estimating the values for critical evaluation parameters such as drug release, drug release kinetics and determine the flaws or defects in tablets etc [46]. AI helps in optimum formulation of tablets with consistency in QC procedures, consuming less time, decreasing efforts, predicting dissolution rates and disintegration time in order to select the best and optimum batch [47-49].

AI skills are also useful in research of nanomedicines whereby AI accelerates the development process of nanoscale therapies, improves diagnostic, provides precise and focused treatment options and improves drug delivery that revolutionize the healthcare system [50-52]. AI algorithms also help in estimating the physiochemical properties, stability and efficacy of drug loaded nanoparticles, nanoparticle behavior, drug release kinetics and toxicity if any [53]. The data from Artificial intelligence can be useful in selection of medication, excipients, dosage form and stimuli responsive material required for formulation of nanoscale medication in treatment of cancer [54]. The AI based computational methodologies are essentially utilized in evaluation of drug loading, nanocarrier formulation stability, drug retention and in vitro drug release kinetics [55]. Several AI based research has been conducted since the development of computational methodologies that includes:

- He et al., 2020 [56] predicted the fate of drug nanocrystals using machine learning. The researchers used Monte Carlo stimulations method to reduce the time and effort in repeating the experiment for preparation of drug nanocrystals employing high pressure homogenization and wet ball milling method. Furthermore, AI database is used for exploring the 3D structure of nanocarrier and evaluating the physiochemical characteristics [57].
- Nuhn L et al., 2023 [58] demonstrated the use of Artificial intelligence in analyzing the transendothelial permeability of nanoparticulate drug delivery system into the tumor site.
- Lin Z et al., 2022 [59] used Artificial intelligence in combination with physiology based pharmacokinetic model in order to conduct the research on tumor medication for effective drug delivery.

Artificial intelligence has also found its applicability in parenteral, transdermal and mucosal route of administration [60, 61]. As with other drug dosage forms here as well AI aids in predicting the physiochemical characteristics of drug dosage form, pH, solubility, rheological properties, and stability. This helps in the formulation of a dosage form with better quality, efficacy and efficiency. AI algorithms ease the way of optimization of injectable formulations that enhance the quality of product, uniformity of product, takes less time, reduce manpower, reduce the chances of batch failures and boost the manufacturing process. It becomes very easy to distinguish the variations and know the pattern of variation in the results obtained for particle size and chromatography which ultimately leads to enhanced quality product with very lesser chances of error that enables the efficiency and reliability of the formulation [62].

In case of parenteral formulations, AI aids in several ways [63]:

- Analyze the particle behavior such as sticking, sedimentation and swimming of particles within the container
- Analyze and process the image for the formulation to evaluate the flaws (bubble formation) if any
- Aids in maintaining the equipments required during manufacturing process such as AI forecast any equipment breakdown and plan maintenance of the same by using the sensor datasets and keep the well maintained record
- AI algorithms assures the product compliance, analyze if there is any incompliance and recommend the research scientist to improve and maintain compliance that ultimately leads to GMP
- Machine learning models such as LGBM has been promising in formulation of Long acting injectables where it reduce the time and cost of the formulation
- Machine learning and Multiscale simulations makes it very accurate in optimizing the formulation that it reduces the trial and error method needed for the manufacturing of ocular, transdermal, pulmonary and mucosal drug delivery systems [64]
- Molecular stimulations, mathematical modeling and pharmacodynamics and pharmacokinetic modeling has reduced the time and effort needed for the development of the formulations [65]

For Pharmacodynamic and Pharmacokinetic parameters

In the process of drug development and manufacturing of drug formulation there are few complicated stages such as drug discovery, preclinical investigation, clinical trials and regulatory approvals that are important part of study but are really tedious and consume high number of manpower [66, 67]. Not only this, these pharmacokinetic and pharmacodynamics parameters when evaluated without any computational techniques do not correctly forecast the safety and effectiveness of the drug [68]. Apart from this, before the concept of artificial intelligence was discovered the studies were conducted on animal and human models that had higher mortality rate or high risk of diseases but nowadays machine learning and artificial intelligence models have not only reduced the models in preclinical and clinical investigation but also reduced the time taken in conducting the study and accurately forecast the pharmacodynamics and pharmacokinetic parameters in an cost effective way [69-71].

Prediction of pharmacokinetic properties: The pharmacokinetic properties such as Absorption, Distribution, Metabolism and Excretion can be evaluated using Machine learning and deep learning models such as Bayesian

Model, Random forest, ANN and Support vector machine. Moreover, the drug absorption, bioavailability, rate of clearance, volume of distribution, and half life of drug can be evaluated using computational techniques such as recurrent neural networks, convolutional neural networks and long short-term memory models. QSAR is also a well known computational technique based on chemical structure of drug molecule used to predict the ADME, drug solubility and drug permeability etc [72-74].

Prediction of Physiologically Based Pharmacokinetic Models: PBPK models are used to stimulate drug distribution and elimination inside the human body that require large amount of datasets and computational techniques. The machine learning models can be helpful in determining the parameters and reducing the high dependency on animal and human models [75, 76].

Prediction of drug release, absorption, metabolism and excretion: The Artificial Intelligence and Machine learning algorithms are also applicable in forecasting the drug release and absorption characteristics by estimating the physiochemical qualities, formulation features, and drug release mechanism. AI is also used to determine the drug release kinetics to know the factors on which the drug release depends. AI models determine the molecular structure and physiochemical properties of the drug molecules in order to predict the drug metabolism and excretion [77-79].

For diagnosis of disease

AI models have been useful in early diagnosis of disease such as cancer [80, 81], hepatitis, Parkinson's disease [82] and dementia. The machine learning, deep learning models, neural networks, and data algorithms are useful in predicting the disease with complete accuracy, sensitivity and specificity [83, 84]. Deep learning is used in prediction of dermatological conditions and artial fibrillation. The decision tree and reasoning models are helpful in prediction of liver diseases. The rib segmentation algorithms and multi-scale networks are essential in predicting lung cancer and pulmonary disorders [85]. AI algorithms and machine learning models are also able to interpret ECG and identify cardiac arrhythmia [86]. Genetic algorithm and support vector machines are useful in diagnosis and classification of Tuberculosis [87-90].

Pros of Artificial Intelligence in Pharmaceutical Research [91-93]

Accelerated Drug discovery: AI models have the potential in accelerating the process of drug discovery by reducing the errors, predicting the results with high accuracy and predicting the structural and chemical behavior of the drug molecules accurately and efficiently [94, 95].

Personalized therapeutic treatment options: AI models can effortlessly store maximum number of data in a personalized way and healthcare workers can easily personalize the medical treatment on the basis of data recorded.

Optimized preclinical and Clinical trials: AI models can reduce the use of animal and human models by optimizing the trials and monitoring at the same time [96, 97].

Drug Repurposing: AI algorithms can be used in identification of new therapeutic use for the old drug moiety by studying the QSAR of the drug and 3D chemical structure of the drug.

Disease diagnosis: AI models have been useful in diagnosis of the disease (cancer, dementia, dermatological disorders & pulmonary diseases) with the help of AI integrated biomarkers including genomics and phenotypic.

Minimize the chances of error: The data recorded and maintained by humans can lead to mistakes and errors but the datasets maintained by AI models and ML algorithms ensures the accuracy of the results with no or minimal error [98].

Time saving and cost effective: AI models give optimized formulations and do not require any trial and error method which ultimately saves times and cost in conducting the experiments.

Cons of Artificial Intelligence in Pharmaceutical Research [99-103]

Despite being advantageous in the field of pharmaceutical research and development, it has few limitations as well that need careful consideration. Artificial intelligence or any computational technique is associated with pharmaceutical R&D hence it is necessary to enlist the limitations of AI to ensure the safety and efficacy of the drug molecules.

***Limited data availability**:* AI models give accurate and unbiased results for evaluation parameters on the basis of datasets available. However, in case of any rare disease or specific population the limited availability of data leads to baised or less accurate results.

***Data biasness**:* AI models require complete, accurate and unbiased data for the accuracy in predictions. If the data is incomplete or inaccurate it can result in errors in predictions carried out for drug molecules. Hence, it is important to ensure that the data provided should be accurate, unbiased and trustworthy as any minor error in the R&D of drug molecules can be fatal in human beings.

Inability to update AI models: AI models works accurately when same drug or similar process in used everytime but if any new drug development process is carried out it is necessary to update the data in AI models. This updation is crucial to get accurate predictions and flawless decision making but the method is very time consuming and costly. Moreover, updating the AI models every now and then is very difficult that can lead to inaccurate predictions.

Top 10 Pharma Industries using AI [29]

1. *Pfizer:* Pfizer collaborated with IBM Watson in 2016 for the new drug discovery in the field of Immuno-oncology. In 2018, Pfizer again collaborated for the advancements in Artificial intelligence. Also, Pfizer announced about its membership with Machine Learning for Pharmaceutical Discovery and Synthesis in a Consortium held at Massachusetts Institute of Technology. Pfizer also partnered with Chinese startup company “Xtalpi” for experimenting in the field of molecular stability and drug designing.
2. *Roche:* Roche designed the Machine learning technique for diagnosis of diabetes macular edema (thickening of retina leading to blindness). In general, Roche utilize the vast clinical trial database to develop AI algorithm to diagnose disease, disease progression and respond treatment in a personalized way.
3. *Novartis:* Novartis in collaboration with AI has the ability to decode cancer images. Novartis collaborated with Tech startup “PathAI” in order to create a system for diagnosis of cancer.
4. *Johnson & Johnson:* Johnson & Johnson used the AI algorithms and machine learning models to predict that patients diagnosed with nonvalvular atrial fibrillation taking Xarelto have fewer risk of strokes when compared to patients administered with Warfarin.
5. *MSD:* Merck and a Spanish Telecome business company Telefonica collaborated for the programme “Velocity” that works on diagnosis and prevention of diabetes and cancer.
6. *Sanofi:* Sanofi collaborated with Recursion Pharmaceuticals for drug repurposing for the new drug molecules that are under clinical stage for many of genetic diseases.
7. *Abbvie:* In 2016, Abbvie collaborated with Aicure to monitor the patients accurately in Schizophrenia Phase 2 trials. Also, Abbvie is working in a confidential project with Atomwise.
8. *GSK:* GSK is working very actively with AI models and is known to have its own AI laboratory “Medicines Discovered Using Artificial Intelligence” which is now named as “In silico Drug Discovery Unit” with almost 50 members.
9. *Amgen:* Amgen has collaborated with a startup company “GNS Healthcare” and machine learning startup “Owkin”. Amgen announced about its membership with Machine Learning for Pharmaceutical Discovery and Synthesis in a Consortium held at Massachusetts Institute of Technology.
10. *Gilead Sciences:* In 2019, Gilead announced its collaboration with AI in drug discovery. In 2022, Gilead also announced its collaboration with AI startup “Insitro” that will work on nonalcoholic steatohepatitis.

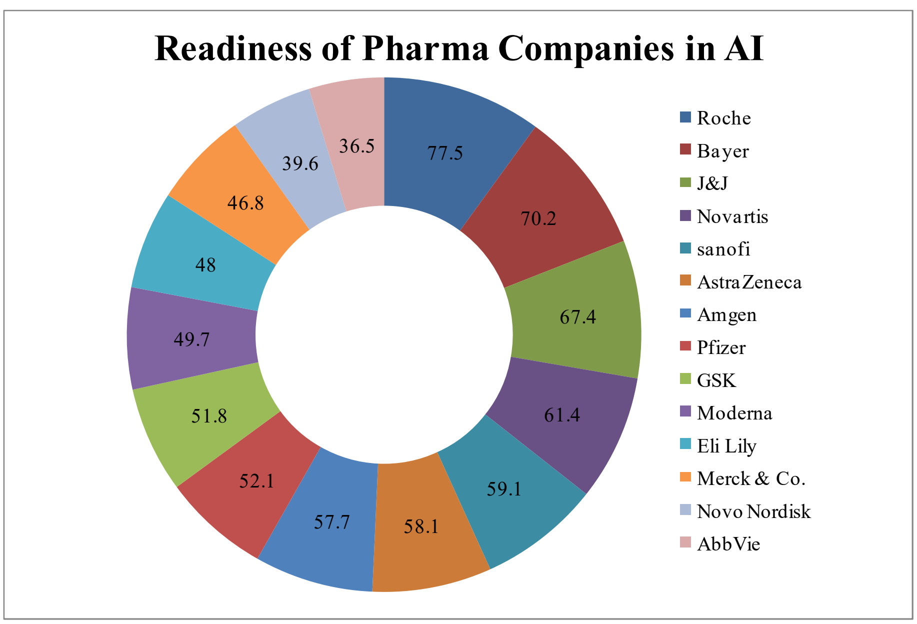

Fig 2: Readiness of AI by top Pharmaceutical Companies as of 2023
(Source: Statista)

CONCLUSION

To conclude, Artificial Intelligence is necessary to transform therapeutic delivery and medicinal technology by providing targeted and personalized medical therapy. AI-based models for pharmaceutical R&D have been useful in drug discovery, drug repurposing, minimizing preclinical and clinical trials, dosage form design and disease diagnosis. The AI technology has significance for its high speed, effective cost, accurate results prediction, improved patient outcome, personalized medicinal therapy and revolutionize the pharmaceutical sector.

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