INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

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Review Article

Artificial Intelligence And Its Integration In Pharmacy

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ARTICLE INFO

Published: 15 Oct 2024

Keywords:

Artificial Intelligence, Pharmaceutical Industry, Drug Discovery, Machine Learning, Deep Learning, Pharmacy Practice, Disease Identification

DOI:

10.5281/zenodo.13936314

ABSTRACT

In recent years, the integration of Artificial Intelligence (AI) into various aspects of the pharmaceutical pipeline has emerged as a game-changing trend, revolutionizing the way we approach drug discovery, clinical trials manufacturing, and personalized medicine, and patient care. This review explores AI's role in pharmaceuticals, highlighting its basic concepts, tools, and applications. AI algorithms analyze biological data, predict disease interactions, and optimize drug development processes. Machine learning techniques, such as supervised and unsupervised learning, are employed in drug design, synthesis, and testing. Deep learning models, including convolutional neural networks and recurrent neural networks, are used for image analysis, protein structure prediction, and genomic data analysis. AI integration in pharmacy practice enhances efficiency, reduces errors, and improves patient care. AI assists in disease identification, diagnosis, and personalized treatment plans. Applications include rare disease diagnosis, gastrointestinal inflammation detection, and oncology diagnostics. This review demonstrates AI's potential to transform the pharmaceutical industry, accelerating innovation, improving efficiency, and enhancing patient outcomes.

INTRODUCTION

Artificial Intelligence is an amalgamation of cognitive processes within the realm of computer science, empowering machine to carry out the tasks effectively. It is the cutting edge technology that enables the machines to replicate the effective functions of the humans. The science or the field of creating the intelligent machines was termed "artificial intelligence" by John McCarthy at a Dartmouth Conference in 1956. Artificial intelligence involves the use of automated algorithms to perform the several tasks typically required for the human intellect. [1] By combining computer-aided design, development, and algorithms, this technology simulates human thought processes, enabling capabilities like machine learning, predictive analytics, and

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

intelligent problem-solving. [2] Artificial intelligence encompasses various fields such as mathematics, linguistics, computer science, psychology, neuroscience and more. [3] AI algorithms can analyze vast amounts of biological data, including genomic and proteomic information, enabling researchers to pinpoint disease-related targets and forecast their responsiveness to potential treatments. [4] It involves the development of machines which can learn, think, plan and mimic the human intelligence. [5] The pharmaceutical industries observed that around 41% of supply chain disruptions occurred in June 2022. [6] 1. A recent report highlights the remarkable advancements of AI in pharmaceuticals over the past five years, while also underscoring supply chain disruption as a critical issue, amplified by the pandemic's far-reaching impact on clinical trials. [7] Disruptions in the pharmaceutical industry's supply chain have notable implications for customer satisfaction, corporate reputation and potential profits. Therefore, integration of Artificial intelligence is poised to revolutionize how the pharmaceutical industry manages its supply chain operations. [8]

Numerous pharmaceutical companies are exploring the integration of never technologies including platforms such as Artificial intelligence. Artificial intelligence utilizes methods to efficiently gather extensive data generated from clinical trials, thereby minimizing the manpower required for the data collection. With the storage of data in machine system, scientists and researchers have gained increased efficiency and competence. Currently, most of the pharmaceutical companies are embracing the AI to get the introduction of new discoveries to the market. An example of such a company is Eli Lilly, which is actively investing in artificial intelligence technologies. One company is employs AI to create novel drugs, while another utilizes AI for screening existing drugs to uncover potential new applications. [9]

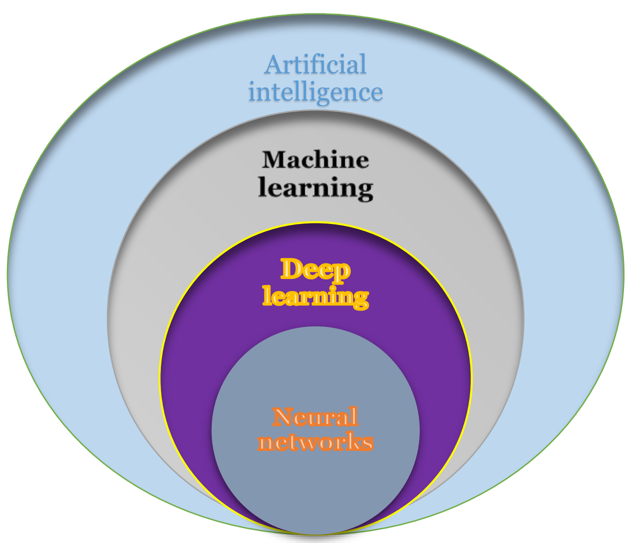

Fig 1: Basics of AI

Basic concepts of Artificial intelligence:

The artificial intelligence involves the basic concepts like machine learning, deep learning and neural networks.

1 Machine learning:

Machine learning is a type of artificial intelligence that concentrates on building algorithms and models, enabling computers to acquire knowledge, predict outcomes, and make data-driven decisions. Machine learning techniques are gaining the part of Al in the drug development industry, because of their automated processes, predictive capabilities, and efficiency improvement. [10] The Development of a new drug is a lengthy and expensive process with a low success rate as evidenced by the following estimates: that indicates an average Research and Development investment is $ 1.3 billion per drug. The median development time for each drug ranges from 5.9 to 7.2 years for non- oncology drugs and 13.1 years for oncology drugs. Additionally, the proportion of all drug development programs that eventually lead to approval is relatively low, standing at 13.8%. [11] Given the challenges in the drug-development, the drug industry finds AI and ML techniques appealing due to their capabilities. These technologies offer the potential to enhance efficiency, reduce costs, and improve success rates in the complex process of bringing new drugs to market.

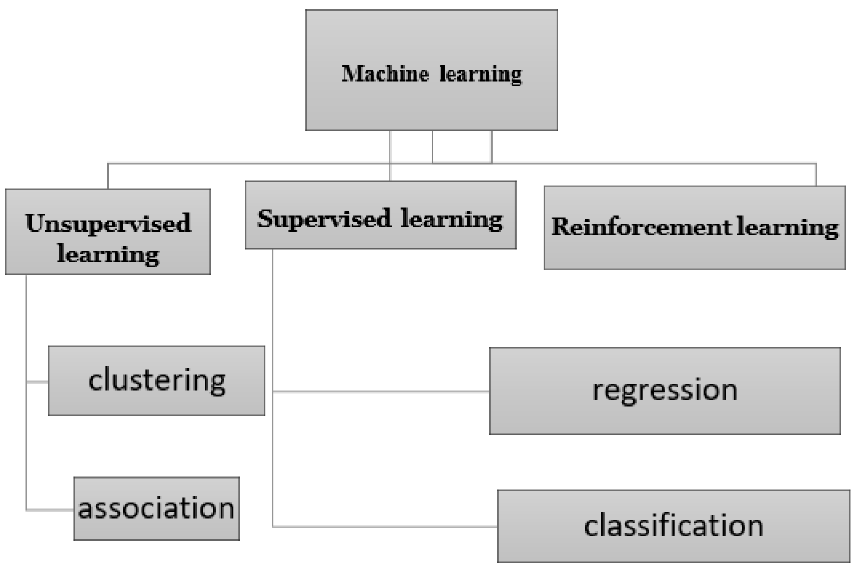

Fig 2: Classification of Machine learning.

1. **Unsupervised learning:**

Unsupervised learning algorithms are applied to determine various classes or clusters within the applied dataset based on similarities without using prior information about class labels. Unsupervised learning, the pharmaceutical industry can uncover hidden patterns and relationships within datasets, ultimately leading to more informed decision making in drug development, manufacturing and marketing. In context of pharmacy, unsupervised learning can be applied in various ways:

a Clustering
b Anomaly detection
c Association rules
d Dimensionally detection

a. Clustering:

Identifying patterns or grouping similar data points together without predefined categories. This can be useful in patient segmentation based on medication response or disease diagnosis.

b. Anomaly detection:

Unsupervised learning can help identify unusual patterns or outliers in pharmacy data, which may indicate the errors, fraud or unexpected patient responses to medication.

c. Association:

Association refers to identifying relationships or patterns within explicit labels or predefined categories. [12]

2. Supervised learning:

SL:

These methods solve classification or regression issues. A Supervised learning used for learning relationships connection between the inputs and the outputs. It shows its usefulness in formulation to measure the cause and effects linking between inputs - output. It is subfield of Machine learning that uses labeled datasets to train algorithms that classify data or predict outcomes accurately. Classification involves disease diagnosis while Regression involves the Drug efficiency. In supervised learning models are trained with DMET prediction.

1. Regression:

If there is relationship between the input variable and the output variable, then the regression algorithms are used. The types of regression algorithms are

1. Linear Regression
2. Regression Trees
3. Non- Linear Regression
4. Bayesian Linear Regression
5. Polynomial Regression.

Researchers in academia have utilized regression based algorithms to create a wide range of asset pricing models.

2. Classification:

It is a process of finding a function which helps in dividing the dataset into classes based on different parameters. Through classification, a computer programs learns from a training dataset and subsequently assigns data into distinct categories or classes. In supervised learning, classification is a type of task where the algorithm learns to map input data to specific categories or classes. The algorithm is trained on a labeled dataset, where each input is associated with a corresponding output class. The goal is to learn a mapping from inputs to classes so that the algorithm can accurately classify new, unseen data. Classification problems, such as identifying spam emails, speech recognition, and detecting cancer cells, can be effectively solved using algorithms like decision trees, support vector machines, and neural networks.

Reinforcement learning: -

Reinforcement Learning enables machines to learn from experience, adjusting their actions based on feedback from interactions with their environment. The agent receives feedback in the form of rewards or punishments, guiding it to learn optimal strategies over time. Reinforcement learning RL is commonly used in scenarios where an agent needs to make a sequence of decisions to achieve a goal, such as in game playing, robotics, and autonomous systems. This method focuses on the decision making and excision in which decision making focuses on DE novo drug design while excision involves the experimental design. [12] [13]

3. Deep learning (DL):

It's a type of Machine Learning that draws inspiration from the interconnected structure of the human brain networks, often referred to as artificial neural networks. It is a subfield of machine learning that involves developing multi-layered neural networks. The term "deep" in deep learning signifies the presence of multiple hidden layers between input and output, enabling the model to learn the hierarchical representation of data. Deep learning encounters challenges which data scientists need to take into account while constructing models. Its models can identify complex patterns in pictures, texts, sounds. And other data, leading to accurate insights and predictions. Deep learning works on multiple neural networks of three or more layers and aiming to simulate the behavior of the human brain. It enables the statisticians to learn from vast amounts of data and interpret trends. Hong ET. al. built a

Deep Learning model to predict whether a protein in a bacterium belongs to the type IV secreted effector (T4SE) category. Similar to the human learning model, Machine Learning and Deep Learning models can progressively recognize different features of the data over time. [14]

Tools of Artificial intelligence.

1. Robot pharmacy:

A robotic pharmacy is a facility where automated systems efficiently handle the preparation and dispensing of medications, contributing to accurate and streamlined processes. For the safety of patients, UCSF Medical Center makes use of robotic technology for the preparation and monitoring of medication. The technology has effectively generated 350000 medication doses with negligible error, as stated in their reports. Within the automated system of the pharmacy, the computers first gather medication command electronically from the physicians and pharmacists of UCSF. [15] The Robotics collect, pack and dispensed the individual doses of the pills. The robotic technology possesses the capability to manufacture hazardous chemotherapy drugs for both oral and injectable administration.

2. MEDi robot:

Medicine and Engineering Designing Intelligence robot is designed to interact with the children in the healthcare settings which provide the supporting and distraction during medical procedures. The Child life team utilizes a range of therapeutics tools, with MEDi being one of them, to implement therapeutic interventions that support and comfort the children in healthcare. The community health sciences professor at the University of Calgary in Alberta, Tanya Bearn, served as the project leader for creation of the pain management robot. These Robot works in Texas Hospital. Initiating friendly connections with children, the robot then provides information about what to anticipate during the medical procedure, fostering a reassuring environment, it instructs them on what should be done, how to breathe during the procedure. [16]

3. Erica Robot:

The Erica, developed by Bans of America, is a virtual assistant powered by artificial intelligence. The Al tool relies on natural language processing capabilities to generate responses resembling human language, customers in obtaining the assistance they required. Erica Robot was developed through collaboration with Kyoto University, the Advanced Telecommunications Research Institute International, and the Japan Science and Technology Agency. The Erica robot communicates in Japanese language, exhibiting human like facial expressions and possessing the capability to comprehend and response to inquiries. The Erica Robot is recognized for its aesthetic appeal and impressive intelligence among android. [17]

4. TUG Robot:

TUG robots are autonomous mobile robots designed for material handling and logistics tasks in various environments, including the hospitals, warehouse and factories. They are often used to transport goods, such as medical supplies or packages, efficiently within facility. The TUG Robot was design to navigate around the hospital and handle the transportation of large items like medical supplies, linens as well as prescriptions, meals, specimens and other resources.

The TUG robot is employed in sizable hospitals, tasked with transporting various loads. The TUG robot communicates with elevators, fire alarms, automatic doors and sensors to navigate through the hospital corridors. [18]

Commonly Used AI models in the pharmaceutical Industry.

a. Generative Adversarial Networks (GANs):

Generative Adversarial Networks (GANS) are a class of ML that consists of two neural networks, namely generator and a discriminator, engaged in a competitive learning process. It finds extensive applications in drug product development for creating innovative chemical structures and enhancing properties through optimization. GANS comprises a generator network responsible for crafting new molecules and a discriminator network that assesses their quality, leading to the generation of structurally diverse and functionally optimized drug candidates. [19]

b. Recurrent Neural Networks (RNNs):

RNNs are frequently employed in tasks related to drug development, including predicting protein structures, analyzing genomic data and designing peptide sequences. Recurrent neural networks (RNNs) have been employed in de novo synthesis, which process sequential information to generate novel molecular structures. It generates chemical structures by SMILES (Simplified Molecular Input Line Entry System) strings, which are compact and human readable way to represent chemical structures. It can assist in drug discovery by analyzing molecular structures. It has also application in prediction of medication adherence. [20]

c. Convolutional Neural Networks(CNNs):

Convolutional neural networks CNNs are a class of deep learning models specifically designed for tasks involving grid structured data, such as images and videos. It demonstrates effectiveness in tasks centered around images, encompassing the analyzing molecular features and identification of drug targets. It has found extensive application in field of medical sciences for radiological images, leading to precise disease diagnosis and providing support for informed decision making. These networks are utilized for predicting structural images of and receptors, achieving accurate protein structure predictions, and contributing to genomics and advancement in medical robotics. It also helps in target identification. [21]

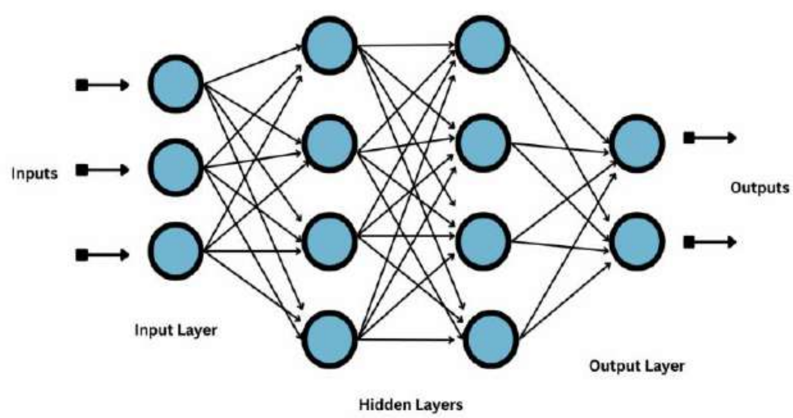

Fig 3: Convolutional Neural Networks(CNNs)

d. Long Short Term Memory Networks: -

LSTM networks are a type of RNN that have been used in pharmacokinetics and pharmacodynamics studies to predict drug concentration time profiles and evaluate drug efficacy. These are designed to capture and remember long range dependencies in data, making them effective for various tasks such as sequence modeling and time series prediction. [22]

e. Transformer Models:

Transformer models are a type of neural networks architecture that excels in handling sequential data by utilizing self-attention mechanisms. These models can extract valuable information from the scientific literature, patent databases and clinical trial data, empowering researchers to make informed decisions in drug development. [23]

f. Bayesian Models:

Bayesian networks and Gaussian processes are employed for decision making in drug development. They enable researchers to make probabilistic predictions, assess risks, and optimize experimental designs. [24]

g. Deep -Q-Networks (DQNs):

DQNs is the combination of deep- learning and reinforcement learning algorithms, typically convolutional neural networks (CNNs) used to optimize drug discovery processes by predicting the activity of compounds. It employs a target network. [14]

h.Graph Neural Networks (GNNs):

GNNS are class of neural networks designed to works with graph structured data. Key components of GNNs include message passing between nodes, graph pooling operations and graph convolutional layers. They can predict properties and aid in virtual screening and de novo drug design. [25]

Applications of Artificial intelligence.

Here's a comprehensive list of AI applications in the pharmaceutical industry:

i. Research and development
ii. Clinical Trials
iii. Manufacturing and supply chain
iv. Regulatory Compliance
v. Marketing and sales
vi. Pharmacovigilance
vii. Patient Engagement

1. Manufacturing:

The boring tasks are possible with the help of robots. Dispensing of acids, mixing, heating, centrifuging and filtering are handled by use of robot. Using a Robotic arm, sample preparation for processes like NMR is now possible. In manufacturing, AI is used for process optimization, predictive maintenance, quality control, and automation.

Machine learning algorithms analyze production data to identify patterns and anomalies, helping optimize workflows and reduce downtime through predictive maintenance. AI-powered robotic systems enhance automation by performing tasks like assembly and material handling. Quality control benefits from computer vision and machine learning, ensuring products meet specific standards. Overall, AI in manufacturing contributes to increased efficiency, cost savings, and improved product quality. [26]

2. Synthesis of Drugs using Al

In the production area of the pharmaceutical industry, the various drugs are synthesized. The various methods are applied for synthesis of Drug. The retrosynthetic procedure stands out as relevant method for synthesis of drug with the incorporation of AI. The retro synthetic pathways can be executed through the application of Artificial intelligence and machine learning, aiding in the analysis of synthetic methods. The development of new drug involves four key Stages. I.e. Design, Fabrication testing and analysis. The artificial intelligence accelerates the new drug research and development cycle by speeding up the discovery of a new synthetic route for target molecules. [27] CASP initially proposed by Corey in 1960s (Computer Aided Synthetic Planning) has benefited from machine learning, contributing to the recent emergence of computer aided synthetic planning in market. [28] Retrosynthetic analysis employs a systematic set of principles in the development of reaction by working backwards from a target compound. Researchers have utilized Artificial intelligence for the prediction of reaction conditions aiming to reduce the time spent on screening various reaction conditions. Coley et al, introduced a neural network model for predicting reaction outcomes, they trained the model with 15,000 reaction examples extracted from the USPTO literature. The robot models analyze samples by using nuclear magnetic resonance and infrared spectroscopy, coupled with machine learning for decision making. [29] Coley et al, introduced a neural network model for predicting reaction outcomes, they trained the model with 15,000 reaction examples extracted from the USPTO literature. [30]

3. AI in Rare Disease Diagnosis.

More than 80% of rare diseases affects fewer than one patient in million. The machine learning and deep learning technology of AI can assist physicians in diagnosing rare genetic conditions by taking photographs of patients Faces.

Some of examples of rare diseases are as follows:

- Eosinophilia-Myalgia Syndrome
- Eosinophilia fasciitis
- Feity syndrome
- Pediatric fibro dysplasia
- Relapsing Polychondritis

Scientists estimate there are more than 7000 rare diseases in total including the conditions like cystic fibrosis, muscular dystrophy. For machine learning applications in diagnosing of rare disease, the variables "medication application" and "type of algorithm" categories were defined. [31]

Type of algorithm used in rare diseases is as follows:

- ANN
- Bayesian methods
- Discriminant Analysis
- Clustering
- Decision Tree
- Regression

Artificial intelligence contributes to rare disease diagnosis by assisting in image recognition, facilitating genetic analysis, providing decision making support. Machine Learning can detect the pulmonary function better than HRCT High resolution computerized tomography and pulmonary function Test.

Deep Learning excels in superior recognition which uses its visible layer to read the image and its hidden layer to extract crucial features from the image, contributing to the precise and accurate diagnosis. Nearly 80 percent of rare disease is genetic. PhenIX, utilizes the Disease associated Genome, which combines phenotypic concepts with genetic information to diagnose Mendellian diseases. Bayesian type of AI models, such as Bayesian comorbidity networks, helps to identifying rare disease patterns. AI not only assists in diagnosing rare diseases but provides essential insights for well- informed clinical decision making.

1. Data analysis -medical data, genetic, clinical
2. Image Recognition - MRI, CT scans, X-rays
3. Genetic Analysis - Identifying rare genetic mutations associated with specific disease.
4. Patient Records and Electronic Health records (EHRs)
5. Clinical Decision support [32]
6. Integration of Artificial intelligence in modern pharmacy practice:

AI integration in pharmacy involves automating tasks which enhances efficiency, reduce errors, and allows pharmacists to focus on patient care.

These are as follows:

1. Medication reminders
2. Drug interactions
3. Patient communications
4. Adverse Drug Reaction monitoring
5. Personalized medication management
6. Electronic health record EHR integration
7. Chronic Disease management
8. Patient education
9. Data analytics
10. Patient screening
11. Telemedicine support
12. Medication adherence tracking
13. Medication therapy management
14. Medication dosage adjustment
15. Patient -centered care. [33]

4. Artificial intelligence in Disease identification:

AI is making significant strides in disease identification across various medical fields. Machine learning algorithms can analyze medical data, such as images, genetic information, and clinical records, to assist in the identification and diagnosis of diseases. For example, AI is being used in medical imaging for early detection of conditions like cancer through radiology or pathology images. Furthermore, AI-powered models can analyze patterns and risk factors, contributing to the prediction and prevention of diseases. Integrating AI into healthcare systems helps in faster and more accurate disease identification, allowing for timely interventions and personalized treatment plans. Artificial intelligence is used in oncology, endocrinology, and neurology diagnostics and therapies development in the berg which is the biopharmaceutical business in United States. [18]

It is extensively applied to identify gastrointestinal inflammation and non-malignant lesions such as ulcers, inflammatory bowel disease (IBD), lymphangiectasia, celiac disease, hookworm infection.etc. AI-based techniques could be of immense support for clinicians in identifying, analyzing, and supporting decision-making through endoscopic images of this disease. A variety of ML methods have been applied to the wireless capsule endoscopy image datasets to detect recurrent bowel bleeding and mortality estimation. In an attempt to accurately identify the bowel bleeding from wireless capsule endoscopy images, numerous models were developed using SVM algorithms. Significant improvements in the prediction accuracies, ranging from 94%-99.2%, are reported by various SVM models.AI algorithms are also widely applied to identify hepatitis B and hepatitis C virus-associated fibrosis. SVM, k-Nearest Neighbors (kNN), Linear regression, Bayesian network, Decision tree have been used to identify the fatty liver disease. [34]

5. AI in Disease Treatment:

Electronic Medical records store securely patient data by using machine and deep learning .ML algorithms can use data contained in EMRs to provide real time estimates for diagnostic purposes and treatment of that disease. Different AI models are utilized in disease like tuberculosis, cardiovascular symptoms. CADD is applied for tuberculosis drug research, the data mining and docking approaches are also applied to available TB genome. [35]

FUTURE DIRECTIONS:

As AI technology continues to evolve, its potential to transform the pharmaceutical industry will only grow. Future research should focus on:

1. Developing more sophisticated AI models for disease diagnosis and prediction
2. Integrating AI with other emerging technologies, such as block chain and IoT
3. Addressing ethical and regulatory concerns surrounding AI adoption
4. Enhancing AI-driven personalized medicine approaches

Implications:

The adoption of AI in pharmaceuticals has significant implications for:

1. Improved Patient outcomes
2. Reduced healthcare costs
3. Enhanced research and development efficiency
4. Increased accessibility to healthcare services

In conclusion, AI has become an indispensable tool in the pharmaceutical industry, driving innovation, efficiency, and improved healthcare outcomes

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HOW TO CITE: Triveni N Gore , Amit J Gatkal, Artificial Intelligence And Its Integration In Pharmacy, Int. J. of Pharm. Sci., 2024, Vol 2, Issue 8, 821-832. https://doi.org/10.5281/zenodo.13936314