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Artificial Intelligence in Pharmacy: Revolutionizing Healthcare and Drug Development

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ABSTRACT

In the pharmaceutical industry, artificial intelligence (AI) is a game-changer, transforming clinical decision-making, patient care, and drug development. Using generative models, deep learning, and machine learning, artificial intelligence (AI) improves pharmaceutical operations' accuracy, efficiency, and cost-effectiveness. AI's various applications in pharmacy are examined in this paper, which also describes its classifications by capabilities (Artificial Narrow Intelligence, General Intelligence, and Super Intelligence), functionalities (reactive machines, limited memory systems), and learning techniques (machine learning, deep learning). Important fields include drug research, where AI speeds up molecular design, virtual screening, and target identification, slashing development times from 14 years to months and drastically lowering costs.

In clinical practice, AI helps with medication interaction monitoring, individualized treatment regimens through EHR data analysis, and illness diagnosis (e.g., Alzheimer's prediction by MRI analysis, cancer detection in dermatology). AI also makes remote patient monitoring and telemedicine more efficient, allowing for early intervention and real-time health tracking. AI-powered technologies (like AlphaFold2 and DeepChem) and databases (like PubChem and Drug Bank) help the pharmaceutical business by streamlining post-market surveillance, clinical trial optimization, and medication creation.

AI is also used in specialist sectors including infectious diseases, cardiology, and cancer to enhance treatment results and diagnosis accuracy. Implementation issues are examined together with ethical issues and future possibilities, such as the potential of artificial general intelligence (AGI). Accelerated innovation, better patient outcomes, and sustainable healthcare solutions are achieved by the industry by incorporating AI into the whole drug lifecycle, from preclinical research to commercialization. This thorough analysis emphasizes how important AI is to bringing pharmacy into the data-driven, patient-centered era.

Keyword: Artificial Intelligence, Pharmacy, Drug Discovery, Machine Learning, Personalized Medicine, Clinical Trials, Medication Adherence, Automation, Healthcare Technology.

INTRODUCTION

Artificial intelligence (AI) is a branch of research that focuses on intelligent machine learning, mostly intelligent computer programs that produce outcomes that are comparable to the attention process of humans[1]. A collection of intelligent behaviours and processes, artificial intelligence (AI) is created by computer models, algorithms, or a set of rules that enable a machine to replicate human cognitive processes like learning and problem-solving[2]. This procedure often entails gathering data, creating effective mechanisms for applying the data, displaying precise or near-exact results, self-corrections, and modifications[3]. The well-known example of an AI-controlled system is Apple's SIRI, which is found in the iPhone Amazon’s Alexa [4]. ChatGPT, a language model-based chatbot by Open AI. In day-to-day living,

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artificial intelligence (AI) is crucial. Significant advancements have been made in a wide range of fields, including natural language processing, picture and speech recognition, and more[5].

AI plays an important role in pharmacy field. Patients' quality of life can be enhanced by artificial intelligence by influencing their behaviour when seeking medical attention and helping them comprehend their symptoms[6]. Even more effectively than human experts, AI assistants have recommended medications for cancer patients[7]. AI technology has recently emerged as a key component of industry for its practical applications in numerous technical and scientific domains. The recent push to embrace AI applications in pharmacy, such as drug delivery formulation creation, drug discovery, and other healthcare applications, has already moved from hype to optimism. Predicting in vivo reactions, therapeutic pharmacokinetic characteristics, appropriate dosage, etc., is also made possible by the application of AI models. Given the significance of drug pharmacokinetic prediction, in silico models are used to increase the efficacy and affordability of drug research. There are several chemicals available from pharmaceutical companies that may be able to treat a wide range of specific disorders. The businesses, however, lack the resources necessary to identify themselves as such. The process of developing and producing new drugs is not simple; it can take a pharmaceutical business up to $2.6 billion and take 12–14 years to complete. This is where pharmaceutical businesses can benefit from artificial intelligence. AI shortens the time required for medication development, which lowers associated costs, increases returns on investment, and could potentially result in lower end-user costs[8]. In silico Medicine revealed Pharm AI, the company's AI initiative. According to Insilico Medicine, they used reinforcement learning algorithms and Generative Adversarial Networks (GAN). One kind of generative model that can both create samples and learn from training examples is the GAN. They consist of the discriminator, the generator, and two neural networks. "Adversarial" describes the interaction between the discriminator and the generator. The discriminator identifies the samples as real or fake after the generator attempts to make and learns to create new samples. Real samples are those that are part of the data set, while "fake" samples are those produced by the generator. As the discriminator improves at the identification process, the generator starts to produce samples that resemble the genuine ones through ongoing training. In silico Medicine asserts that it can create novel molecular structures and speculate on the biological cause of an illness using Pharma AI, GAN, and reinforcement learning[9].

Figure 1: AI in pharmacy

Classification of AI:

Artificial Intelligence (AI) has improved patient care, medication development, distribution, and discovery, among other pharmacy-related areas. Artificial intelligence (AI) in the pharmaceutical industry may be categorized according to its features and capabilities, which is similar to generic AI classifications but customized for certain pharmacy applications.[10]

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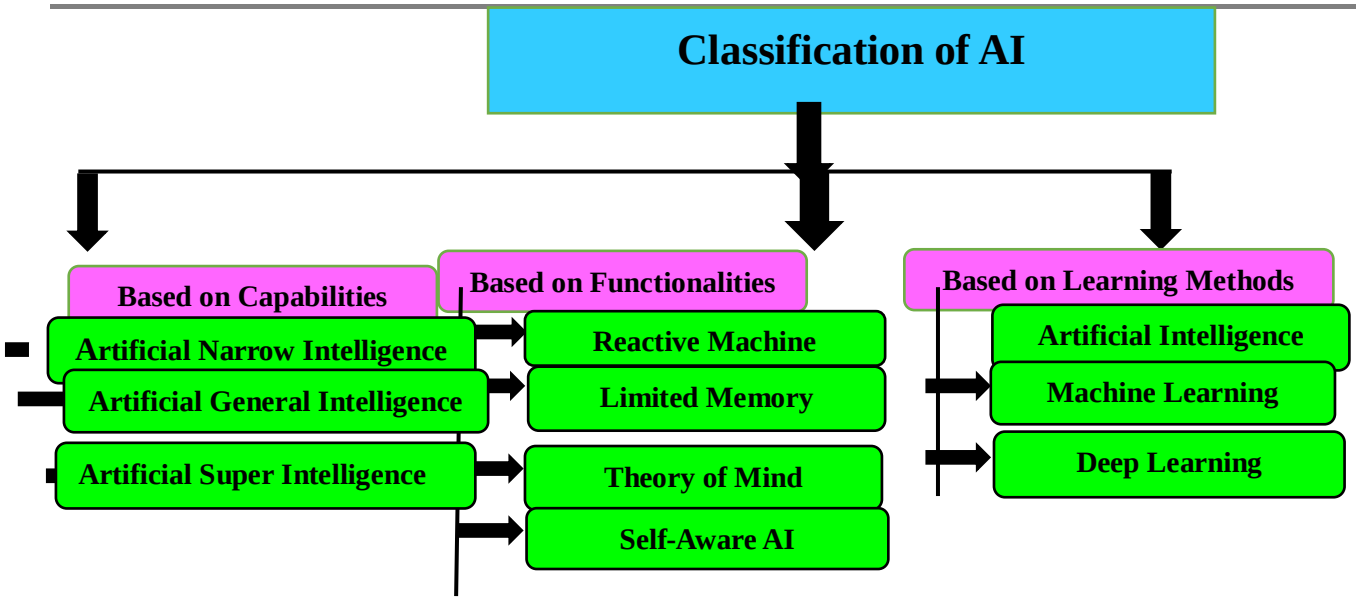

Figure 2: Classification of AI

Based on Capabilities:

Artificial Narrow Intelligence (ANI): ANI in pharmacy refers to AI systems intended to carry out certain functions such anticipating drug interactions, refining drug formulations, and evaluating patient information to suggest individualized prescription schedules. These systems are essential to many pharmaceutical procedures and function within predetermined parameters.

- **Artificial General Intelligence (AGI):** AI systems that can understand, learn, and apply information across a wide range of pharmaceutical activities, from drug research to patient counseling, would be considered artificial general intelligence (AGI) in pharmacy. However, AGI has not yet been applied in pharmaceutical practice and is currently in the research stage.
- **Artificial Super Intelligence (ASI):** Hypothetical AI systems known as ASIs are thought to be more intelligent than humans in every field, including medicine. The creation of ASI continues to be a theoretically debated topic and brings up a number of ethical and practical issues.

Based on Functionalities:

- **Reactive Machines**: AI systems that analyse patient data to find possible drug-drug interactions and improve patient safety might be considered reactive machines in the pharmaceutical industry[11].
- **Limited Memory:** Artificial intelligence (AI) systems in pharmacies with limited memory can use past patient data to forecast medication reactions and enhance treatment regimens, enhancing therapeutic results.
- **Theory of Mind:** Although it hasn't been implemented yet, AI with a theory of mind in pharmacy would include programs that can comprehend and interpret human intents and emotions, which might improve interactions between patients and pharmacists as well as provide more individualized treatment.
- **Self-Aware AI:** In complicated pharmacological circumstances, this enhanced AI would be able to make judgments on its own since it would be capable and self-aware. Still, there is a lot of study and discussion about self-aware AI.

Based on Learning Methods:

- **Artificial Intelligence:** AI systems that mimic human learning, understanding, creativity, problem-solving, decision-making, and autonomy fall under this category. AI technology makes it possible for robots to carry out operations that normally demand for human intelligence.

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- **Machine Learning (ML):** Machine learning (ML), a branch of artificial intelligence, uses algorithms to let computers learn from and make judgments based on data. In contrast to classical AI, machine learning (ML) systems get better over time as they are exposed to more data.
- **Deep Learning:** Deep learning is a branch of machine learning that uses multi-layered neural networks to model intricate patterns in data. Particularly, it works well in voice and picture recognition.
  These divisions offer a framework for comprehending the many uses and phases of development of AI technologies in the pharmaceutical sector, focusing both present-day potential and future opportunities.

Application of AI in Pharmacy

Artificial Intelligence in Healthcare Diagnosis:

In the medical field, early and accurate disease diagnosis remains a difficulty. It might be difficult to identify medical disorders and their symptoms. AI's data processing capabilities can help therapists save time and increase accuracy. By using machine learning, artificial intelligence can significantly help physicians diagnose patients by analysing large amounts of electronic health data (EHRs). AI can assist in early dementia and Alzheimer's disease prediction, for instance, by examining a large number of similar cases and potential therapies[12].

AI may potentially assist physicians in making decisions in emergency rooms and other critical settings. Here, AI systems can shorten wait times and assist prioritize more urgent cases. AI-enhanced decision support systems can help healthcare practitioners make decisions by providing real-time recommendations and quicker data interpretation[13].

AI in Electronic health records

Electronic health records, or EHRs, are essential to the healthcare industry's digitization and information dissemination. Some predict that artificial intelligence will be used to interpret medical records and give doctors new information now that almost 80% of practices use electronic health records. By matching comparable medical phrases, one application employs natural language processing (NLP) to provide more concise reports that reduce variation between medical terms[14]. These variations are combined by NLP algorithms to enable analysis of bigger datasets[15]. NLP may also be used to identify repetitive words in medical notes and retain essential information to make them simpler to read[16].

AI algorithms are capable of more than just editing material in an EHR; they can also assess a patient's record and estimate their likelihood of contracting a disease based on their past data and family history. One type of algorithm is a rule-based system that uses flow charts to make choices, just like people do. This system generates a set of rules that link certain observations to determined diagnoses after ingesting vast volumes of data. As a result, the algorithm may use the data of a new patient to attempt to forecast the likelihood that they would suffer from a certain illness or condition[17]. The algorithms can identify any unresolved concerns to bring to a doctor's notice and save time since they can assess a patient's information based on collection data[18].

AI in Drug interactions

The development of algorithms to detect drug-drug interactions in medical literature was facilitated by advancements in natural language processing[19]. People who take many prescriptions at once run the risk of experiencing drug-drug interactions, and the risk rises as the number of medications taken rises. Machine learning techniques have been developed to extract information on interacting medicines and their potential effects from medical literature in order to overcome the challenge of monitoring all known or suspected drug-drug interactions. In order to provide a standardized test for these algorithms, a group of researchers from Carlos III University compiled a corpus of literature on drug-drug interactions in the DDI Extraction Challenge in 2013[20]. Competitors were assessed on their ability to correctly identify which medications were demonstrated to interact and what those interactions' features were based on the text. This corpus is being used by researchers to standardize the assessment of their algorithms' efficacy[21].

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AI in Telemedicine

The growth of telemedicine, or treating patients at a distance, has shown the potential for AI applications[22]. AI can help provide remote patient care by keeping an eye on patient data via sensors. The capacity to continuously monitor a patient and identify changes that might be harder for people to detect may be made possible by wearable technology. By applying artificial intelligence algorithms, the data may be compared to previously acquired data, alerting doctors to potential risks[23].

Chatbot therapy is another way that artificial intelligence is being used. Yet, other studies argue that using chatbots for mental health treatment does not provide the responsibility and reciprocity of care that should be present in the interaction between the person receiving mental health care and the care provider (whether a psychologist or a chatbot)[24].

AI in Clinical applications

AI in Cardiovascular

Artificial intelligence algorithms have demonstrated encouraging outcomes in correctly identifying and classifying people at risk for coronary artery disease, suggesting that they may be used as a first line of triage[25]. Predicting adverse events, drug side effects, and patient mortality after acute coronary syndrome therapy has been done using several methods[12]. The capacity to monitor cardiac data points in patients has also been demonstrated by wearables, cell phones, and internet-based technologies. This expansion of data and the range of parameters available to AI models may allow for the early diagnosis of cardiac events that take place outside of hospitals[26]. The use of AI to the classification of cardiac sounds and the diagnosis of valvular disease is another rapidly expanding field of study[27].

AI is being utilized more and more in organoid research and cardiovascular tissue creation to incorporate electrophysiological readouts and evaluate microscope pictures[28].

AI in Dermatology

Researchers have found that AI systems can detect cancer more accurately than dermatologists[29]. In dermatology, medical imaging techniques including X-rays and photographs are frequently utilized[30] and image processing has played a significant role in the advancement of deep learning. Therefore, deep learning and dermatology are a perfect match. Processing these photos with machine learning has a lot of promise for improving diagnosis[31].

AI has also been proposed to automatically assess the results of cleft palate treatment or maxillo-facial surgery in terms of age appearance or facial attractiveness[32].

AI in Gastroenterology

AI has applications in several areas of gastroenterology. Rapid identification of aberrant tissue is essential for endoscopic procedures like colonoscopies and esophagogastroduodenoscopies (EGD). Clinical professionals may more quickly detect illnesses, assess their severity, and see blind areas by integrating AI into these endoscopic procedures. Early tests of AI-based early stomach cancer detection systems have demonstrated sensitivity comparable to that of skilled endoscopists[33].

AI can help physicians treat ulcerative colitis identify the microscopic activity of the illness in patients and forecast when flare-ups will occur. To analyse digitalized bowel samples (biopsies), for instance, an AI-powered tool was created. With 80% accuracy, the technology could differentiate between samples with active colitis and those in remission. With the same precision, it forecasted the likelihood of a flare-up occurring. These success rates for forecasting disease flares using microscopic disease activity are comparable to pathologists' accuracy[34].

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AI in Obstetrics and gynaecology

Artificial intelligence makes use of vast volumes of data to assist in patient monitoring, diagnosis, prevention, and sickness prediction. Foetal cardiotocography, ultrasonography, and magnetic resonance imaging are all applications of artificial intelligence in obstetrics. Numerous obstetrical diagnostic problems can be resolved with the use of artificial intelligence[35].

AI in Infectious diseases

In the field of infectious disease medicine, artificial intelligence has demonstrated promise in both lab and clinical settings[36]. AI has been utilized during the COVID-19 pandemic for a variety of purposes, including early identification, tracking the transmission of the virus, and analysing its behaviour[37].

Additional uses of AI in the context of infectious illnesses include enhanced point-of-care Lyme disease diagnostics based on antigen detection, machine learning analysis of blood smears to detect malaria, and support-vector machines that detect antibiotic resistance. AI has also been researched to anticipate treatment problems in patients with hepatitis B and hepatitis C, as well as to improve the diagnosis of meningitis, sepsis, and TB[38].

AI in Neurology

AI technologies have been investigated for application in Alzheimer's disease (AD) diagnosis and prognosis. Using structural MRI inputs, machine learning models have been created for diagnostic applications[39]. These models' input datasets come from sources like the Alzheimer's Disease Neuroimaging Initiative[40]. To increase early diagnosis accuracy, researchers have created models that use convolutional neural networks[41]. Deep learning techniques like generative adversarial networks have also shown promise in the diagnosis of AD[42]. The development of machine learning models into forecasting tools that can predict the prognosis of AD patients has also been attempted. Researchers have suggested generative models for patient outcome forecasting as a way to combine training and validation data[43].

AI in Oncology

AI has been investigated for application in risk assessment, cancer medication development, cancer diagnosis, and molecular tumour characterization. Making precise predictions about which treatment plans will work best for each patient based on their unique genetic, molecular, and tumour-based features is a specific oncologic care problem that AI is being developed to solve[44]. AI has been used to interpret pathology slides and imaging studies in cancer diagnosis trials[45].

Google DeepMind revealed an algorithm in January 2020 that can detect breast cancer in screening scans more accurately than human specialists[46]. According to a July 2020 article, an AI system created by the University of Pittsburgh has 98% sensitivity and 97% specificity, the greatest accuracy to far in detecting prostate cancer[47].

A research from 2023 found that AI could classify CT-based radiomics with 82% accuracy in classifying the aggressiveness of retroperitoneal sarcoma, compared to 44% accuracy for lab examination of samples[48].

AI in Ophthalmology

Artificial intelligence-enhanced technology is being utilized to help prevent blindness and check for eye diseases[49]. In 2018, the U.S. Food and Drug Administration approved the first medical gadget to use an artificial intelligence algorithm to diagnose diabetic retinopathy, a particular kind of eye illness. Furthermore, because AI technology has the ability to shorten detection times, it might be leveraged to further increase "diagnosis rates"[50].

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AI in Pathology

Pathological examination of cells and tissues is regarded as the gold standard for diagnosing many disorders. Digital pathology techniques enable the scanning and digital analysis of microscope slides. A variety of illnesses, such as colorectal cancer, stomach cancer, hepatitis B, and breast cancer, may now be diagnosed with the use of AI-assisted pathology tools. AI has also been utilized to forecast illness consequences and genetic abnormalities. AI is ideal for low-complexity pathological examination of large-scale screening samples, such those for breast or colorectal cancer, which reduces the workload for pathologists and speeds up sample analysis turn around. A number of artificial neural network and deep learning models have demonstrated accuracy comparable to that of human pathologists, and a study on the use of deep learning to diagnose metastatic breast cancer in lymph nodes revealed that the accuracy of human diagnosis when aided by a deep learning software was greater than that of either human or AI diagnosis alone. AI may also detect histological results at levels that are invisible to the human sight. It has demonstrated the ability to more precisely identify the tumour of origin for metastatic cancer by using genotypic and phenotypic data[51].

AI in Pharmacy

The use of artificial intelligence (AI) in pharmacy refers to the process of finding, creating, and administering drugs to patients.AI in pharmacy operations has the potential to improve the clinical use of medications to prevent, treat, or cure disease as well as to completely transform pharmaceutical research in every aspect. Applications for artificial intelligence (AI), a technology that makes it possible for robots to mimic human intellect, include medication delivery systems, clinical trial optimization, pharmaceutical research, treatment regimens, and patient-centered services.

AI in Digital Therapy/Personalized Treatment

In the raw datasets, AI may be able to create a meaningful association that may be used for illness diagnosis, treatment, and prevention. Numerous cutting-edge methods for computational comprehension in this new discipline might be employed in practically every facet of medical research. Extensive knowledge must be acquired, analyzed, and applied to address the complicated clinical concerns[51].

Physicians are now able to solve complex clinical problems with the help of medical AI. Healthcare workers can get help processing data with the use of systems like artificial neural networks (ANNs), soft expert systems, evolutionary computational algorithms, and hybrid intelligent systems. Based on the ideas of the biological nervous system, artificial neural networks (ANNs) are made up of networked computer processors called neurons that can process input in parallel. A binary threshold function was used to produce the first artificial neuron. With its input layer, middle layer, and output layer, the multilayer feed-forward perceptron became the most often used model. Numerical weights are used to connect each neuron. In 1974, Paul Werbos presented a novel method known as "backpropagation learning," which has an appropriate learning algorithm[52].

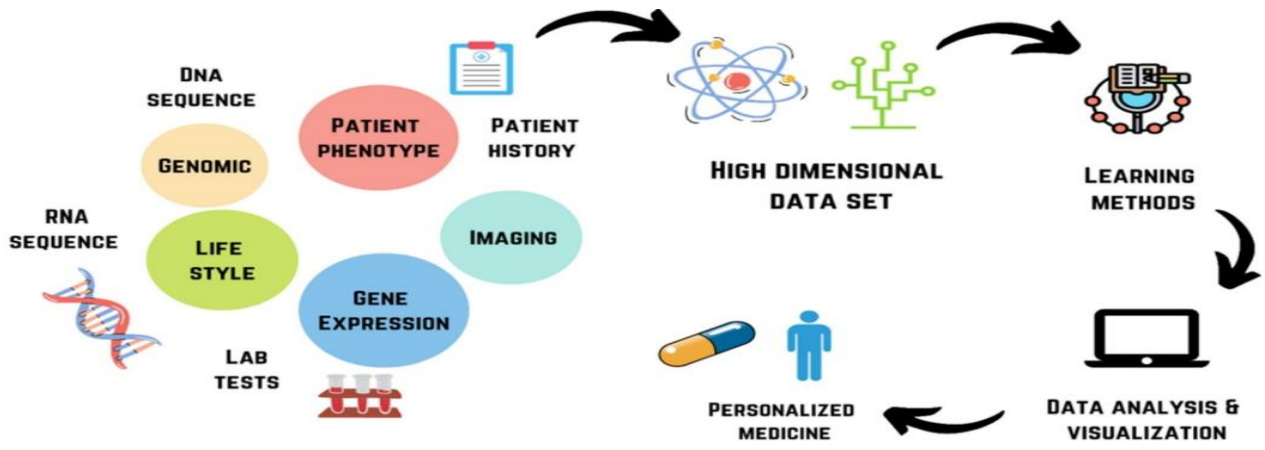

Figure 3: AI in acquiring and analysing data of a patient in personalizing the treatment

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AI in Pharmaceutical Industry:

The pharmaceutical sector has seen changes as a result of artificial intelligence at many stages of drug research, development, and commercialization. AI-driven technologies have greatly improved the drug development process and provided creative answers to the industry's problems. The pharmaceutical business, which may employ automated algorithms to do tasks that traditionally needed human expertise, is one area that looks to benefit greatly from artificial intelligence (AI) technologies and techniques. The pharmaceutical sector has been totally transformed as a result of scientists' use of artificial intelligence (AI) to create new medications, discover ways to treat illnesses, and more[53].

Many pharmaceutical corporations have invested in and formed joint ventures with AI businesses in an attempt to create better healthcare solutions with the rapid introduction of AI in healthcare, particularly in 2016 and 2017. Among these are advancements in biomarkers or diagnostics, the discovery of therapeutic targets, and the creation of novel medications. Modern AI healthcare is moving away from general medicine and toward data-driven treatment[54].

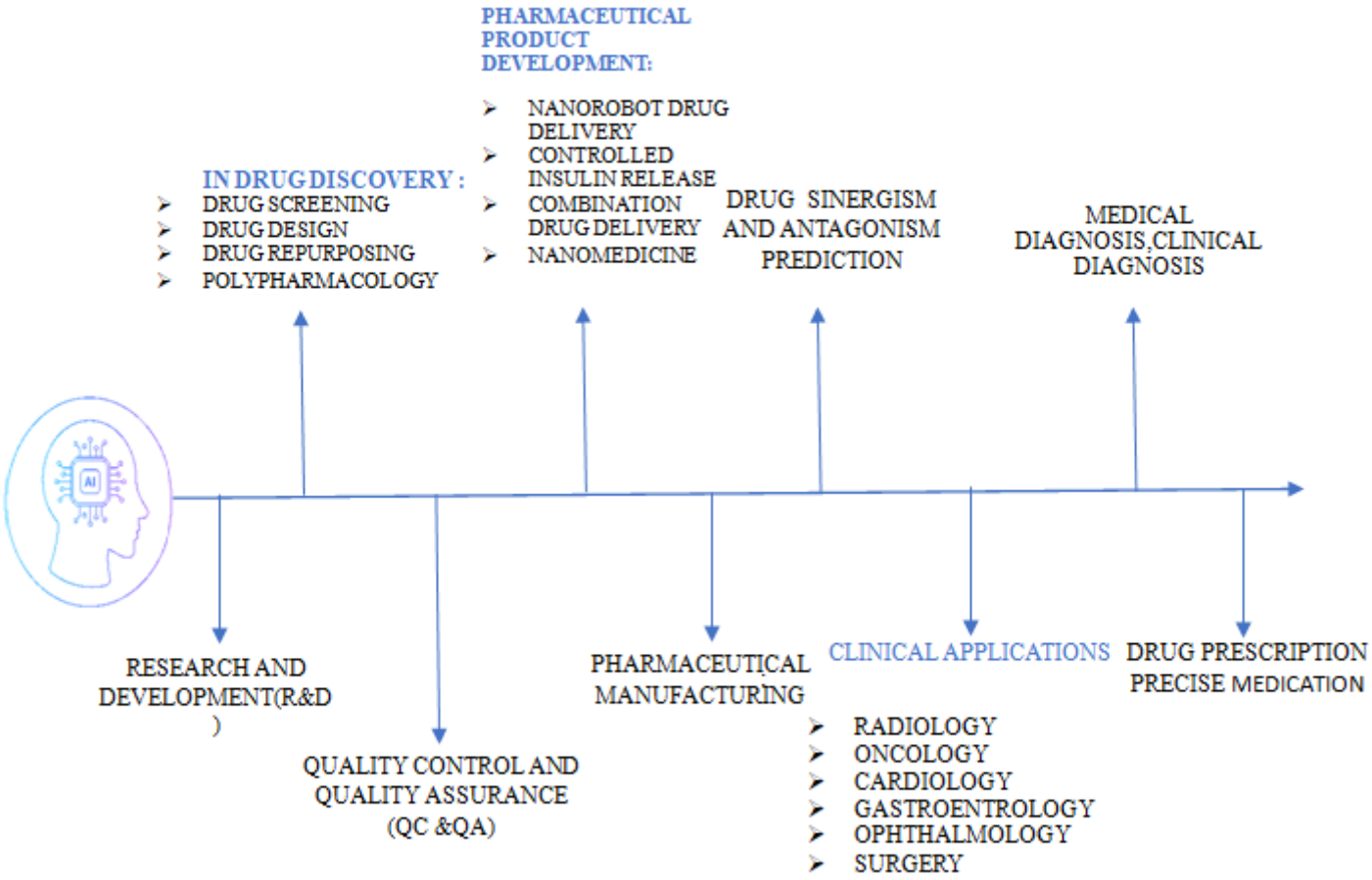

Figure 4: Role of Artificial Intelligence in Pharma sector

AI: a transformative tool for advancing pharmaceutical product lifecycle

Throughout the pharmaceutical product life cycle, from medication research to post-market surveillance, artificial intelligence has become a game-changer. AI has had a significant impact on drug discovery by speeding up the process of finding possible therapeutic candidates. Artificial intelligence (AI) can evaluate large datasets, such as genetic data and chemical attributes, by utilizing machine learning algorithms to forecast the potential interactions and behaviors of various molecules. This speeds up the research process, which drastically cuts down on the time and expenses typically involved in launching a new pharmaceutical product. Clinical trial optimization throughout the development stage is greatly aided by AI[55].

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In order to find qualified trial candidates, anticipate possible side effects, and improve the trial design, machine learning algorithms can evaluate patient data. By ensuring the proper people are enrolled, this increases clinical trial efficiency and improves patient outcomes, producing more solid and trustworthy data. Furthermore, AI may help with the tracking and evaluation of empirical data, offering insights into the long-term safety and effectiveness of medicinal goods[56].

AI for Drug Discovery

The necessity for new medicine development is evident in the rise of pandemics and epidemics like COVID-19 and influenza, as well as the prevalence of serious illnesses like cancer and heart disease[57]. Target discovery, validation, high throughput screening, animal research, safety and effectiveness procedures, clinical trials, and regulatory approval need a multi-stage process that is typically followed.

It takes around 14.6 years and costs roughly US$ 2.6 billion on average to develop a new medicine. Identifying new targets, assessing drug-target interactions, investigating disease processes, and enhancing small molecule compound design and optimization are some of the steps in this process where AI-based techniques might be applied. These techniques may also be used to investigate pharmacological effectiveness, response, and resistance, as well as to find and create predictive biomarkers[58].

AI in pre-clinical and clinical development

One of the most important steps in the drug design process is predicting potential reactions to a medication. The effectiveness of a drug-target interaction and the reaction of a drug on individual cells may be predicted using similarity or feature-based machine learning techniques based on binding affinity or free energy of binding[59].

While feature-based approaches identify unique characteristics of medications and targets and input the drug-target feature vector to the classifier, similarity methods use the assumption that comparable drugs operate on similar targets. Examples of deep learning-based techniques that use convolution and attention mechanisms to learn the embedding of medications and targets include DeepConv-DTI and Deep Affinity[60].

AI in Target Identification

AI algorithms are able to find possible treatment targets by analysing a variety of data sources, including clinical, proteomic, and genomic data. AI helps in drug development by identifying molecular pathways and targets linked to illness that can alter biological processes. A critical first step in developing a treatment plan is accurately determining the target.

Many types of artificial intelligence (AI), including machine learning, neural-based learning, deep learning, and network-based learning, are being used in databases, online services, and apps. These tools make it easier to identify and validate goals, which eventually helps initiatives succeed. This study focuses on the many kinds and subcategories of AI databases used in cancer target identification and drug development[61].

AI in Virtual screening

AI makes it possible to efficiently screen large chemical libraries in order to find therapeutic candidates that are highly likely to bind to a particular target. AI saves time and money by helping researchers prioritize and choose compounds for experimental testing by modelling chemical interactions and forecasting binding affinities[62]**.**

AI integration in virtual screening has a number of benefits, such as increased hit rates when compared to conventional screening techniques, the capacity to forecast ADME/Tox characteristics and "drug-likeness" throughout the screening process, and the opportunity to investigate how all currently available compounds interact with all potential targets. For additional validation, it is crucial to remember that the outcomes of virtual screenings should be supported by relevant laboratory tests and clinical research. The importance of AI-enhanced virtual screening in drug development, especially in the search for anticancer drugs, has been

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cemented. Finding possible anticancer lead compounds from natural sources has been made easier by the capacity to quickly screen natural product libraries, which include alkaloids, coumarins, flavonoids, lignans, quinones, tannins, and terpenes[63].

AI in Structure-Activity Relationship (SAR) Modelling

Artificial intelligence models are able to connect a compound's chemical makeup to its biological action. This enables scientists to create compounds with desired properties, such high potency, selectivity, and advantageous pharmacokinetic profiles, in order to optimize therapeutic prospects[64].

AI in De Novo Drug Design

AI computers can suggest new chemical compounds that resemble drugs by using generative models and reinforcement learning. AI broadens the chemical space and facilitates the creation of novel drug candidates by learning from chemical libraries and experimental data[65].

AI in Optimization of Drug Candidates

AI systems are able to evaluate and improve medication candidates by taking into account a number of variables, such as pharmacokinetics, safety, and effectiveness. This aids scientists in adjusting medicinal compounds to maximize their efficacy and reduce any possible adverse effects[66].

AI in Drug Repurposing

AI methods are able to examine vast amounts of biological data in order to find current medications that could be useful in treating various illnesses. Artificial Intelligence speeds up and lowers the cost of drug research by repurposing current medications for new uses[67].

Artificial intelligence (AI) methods like generative adversarial networks (GANs) and DNNs have demonstrated exceptional promise in the classification of intricate drug action processes, pharmacological property prediction, and the creation of new therapeutic compounds. GANs may create novel molecular structures based on actual data, creating opportunities for creative drug creation, whereas DNNs can group medications into therapeutic categories according to their functional class, effectiveness, therapeutic usage, and toxicity[68].

AI in Drug Bioactivity Prediction

A revolutionary development in the field of drug discovery, especially in the prediction of drug bioactivity, is the use of AI into drug screening procedures. The way scientists evaluate the therapeutic potential and comprehend the mechanisms of action of drug candidates is being revolutionized by artificial intelligence's ability to find new targets by identifying potential interactions and predicting a compound's affinity for particular proteins or receptors[69].

Reference	Description	Link
PubChem[74]	The largest database of publicly available chemical and bioactivity data	https://pubchem.ncbi.nlm.nih.gov/
ChEMBL[75]	A comprehensive database of bioactivity for drug development	https://www.ebi.ac.uk/chembl/
Drug Bank[76]	An informational database about medications, their effects, and their targets	https://go.drugbank.com/

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ZINC[77]	An open-source tool for virtual compound screening	https://zinc.docking.org/
BindingDB[78]	A database that measures the drug's binding affinity to the target	https://www.bindingdb.org/bind/index.jsp
ADME[79]	A website that provides pharmacokinetic data	https://www.fujitsu.com/global/solutions/business-technology/tc/sol/admedatabase/

Drug-target binding affinity (DTBA) prediction is essential for assessing a drug's effectiveness[70]. AI-based approaches use similarity-based interactions, which assume that medications with comparable features would interact with similar targets, as well as feature-based interactions, which take into account the chemical characteristics of both pharmaceuticals and targets. To precisely forecast DTBA, tools like ChemMapper and the similarity ensemble approach (SEA) have been used, in addition to machine learning and deep learning methods including KronRLS, SimBoost, DeepDTA, and PADME. These artificial intelligence techniques provide notable advancements over conventional techniques by employing sophisticated computer models that are independent of the accessibility of three-dimensional protein structures, hence expanding the potential for forecasting drug-protein interactions[71].

AI in FDA approval and post-market analysis

Natural language processing, or NLP, may be used to search scientific literature for reports of pharmacological side effects, such as toxicity or resistance, and to provide automated reviews for FDA clearance or patent applications. Drug recommendations may be made using sentiment analysis techniques based on natural language processing. Pharmaceutical businesses may be able to maximize their business resources by using machine learning-based methods to predict a product's anticipated sales[72].

Existing databases and tools for drug development

Chemical and biological databases

It is necessary to compile data from computationally generated drug-target interactions (DTI) and experimental bioassays into publically accessible databases. Table 1 lists the databases for compounds and bioactivity, whereas Table 2 lists the databases for targets and chemicals[73].

GDSC[80]	Information about drug response and genomic biomarkers	https://www.cancerrxgene.org/
PDBBind[81]	The Protein Data Bank (PDB) has an extensive database of binding affinities for the protein–ligand complexes	http://www.pdbbind.org.cn/
canSar[82]	Translational research on cancer and a knowledge basis for medication development	https://cansarblack.icr.ac.uk/

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Table 1. List of Compound and Bio-activity databases.

Reference	Description	Link
PDB[83]	The Protein Data Bank Archive offers details on the three-dimensional structures of proteins, nucleic acids, and complex assemblies.	https://www.rcsb.org/
UniProt[84]	An open resource of protein sequences and functional information	https://www.uniprot.org/
Atom3D[85]	A comparison of datasets of 3D molecules that are currently available and cover multiple types	https://github.com/drorlab/atom3d
TTD[86]	A database of possible therapeutic targets	http://db.idrblab.net/ttd/
MoleculeNet[87]	A standard dataset for molecular machine learning	https://moleculenet.org/

AI-based software tools for drug development process

Artificial intelligence (AI) technologies have the potential to revolutionize drug development by empowering scientists to quickly evaluate vast amounts of data, create novel compounds, and forecast the effectiveness of possible treatment options. In this article, we examine a few of the most widely used AI technologies for drug development[88]**.**

Table 2. List of Target and Chemical databases.

Reference	DESCRIPTION	Source Code
AlphaFold2[89]	A deep learning-based algorithm for predicting proteins' three-dimensional structures from amino acid sequences	https://github.com/deepmind/alphafold/
DeepChem[90]	Drug development and computational chemistry using a deep learning library	https://github.com/deepchem/deepchem
DeepBind[91]	A computational technique for examining protein-DNA/RNA binding	https://fastmbar.readthedocs.io/en/latest/
Dee0000000pBar[92]	A technique for quickly and accurately predicting binding free energy	https://fastmbar.readthedocs.io/en/latest/
Deep-Screening[93]	A deep learning-based web server for virtual compound screening	http://deepscreening.xielab.net/
Deep Screen[94]	High-performance drug-target relationships	https://github.com/cansyl/DEEPScreen
DeepConv-	A model for forecasting drug-target	https://github.com/GIST-

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DTI[95]	interactions based on convolutional neural networks	CSBL/DeepConv-DTI
Deep Purpose[96]	A deep learning collection for predicting protein function, drug-target interaction, drug-drug interaction, and protein-protein interaction	https://github.com/kexinhuang12345/DeepPurpose
DeepTox[97]	To forecast the toxicity of chemical substances, a deep learning model	http://www.bioinf.jku.at/research/DeepTox/
AtomNet[98]	The prediction of bioactivity using a deep convolutional neural network	github
PathDSP[99]	A deep learning technique that uses cancer cell lines to predict drug susceptibility	https://github.com/TangYiChing/PathDSP
Graph level representation[100]	Acquiring knowledge about graph representation for drug discovery	https://github.com/ZJULearning/graph_level_drug_discovery
Chemical VAE[101]	A framework for creating novel compounds based on auto-encoders	https://github.com/aspuru-guzik-group/chemical_vae/
DeepGraphMol [102]	A computational approach that uses graph neural networks and reinforcement learning to create molecules with desired qualities	https://github.com/dbkgroup/prop_gen

Comparison of AI Tools in Pharmacy & Drug Development

Table 3. List of AI-based software for drug discovery, development, and analysis.

AI Tool / Software	Application Area	Key Features	Strengths	Limitations
AlphaFold2	Protein structure prediction	Predicts 3D structure from amino acid sequence using deep learning	Extremely accurate; groundbreaking in structural biology	High computational resource requirements
DeepChem	Drug discovery & cheminformatics	Open-source deep learning library for molecular tasks	Broad scope; customizable; community-supported	Requires programming proficiency
DeepBind	Protein-DNA/RNA interaction	Predicts binding affinity using sequence features	High precision for genomic/proteomic tasks	Limited to nucleic acid-binding predictions
DeepTox	Toxicity prediction	Predicts chemical toxicity using DL algorithms	Helps early safety screening; high throughput	May need further validation for novel compounds
Deep Screen	Drug-target	CNN-based prediction using	Fast and accurate; useful in high-	Focused on specific

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	interaction	2D compound images	throughput screening	representation types
Deep-Screening	Virtual compound screening	Web server using deep learning for hit prediction	Easy to use; useful in natural product libraries	May lack explainability
AtomNet	Structure-based bioactivity	CNN-based platform for 3D molecule interaction predictions	First AI for structure-based screening; high accuracy	Commercial; limited open access
Deep Purpose	Multi-purpose drug modelling	Predicts DTIs, PPIs, DDIs using a unified DL framework	Versatile; supports multiple input formats	Complex setup for beginners
PathDSP	Drug sensitivity prediction	Integrates biological pathway data with drug response	Good for cancer-focused personalized treatment	Early-stage tool; limited generalizability
DeepGraphMol	Molecule generation	Combines graph neural networks with reinforcement learning	Creates novel molecules; learns molecular rules	Requires significant training data and tuning
Chemical VAE	De novo molecule design	Autoencoder-based generative framework for chemical structures	Explores novel chemical space; useful for ideation	Might generate chemically unstable structures
DeepConv-DTI	Drug-target interaction	CNN-based DTI prediction using protein sequences	Learns from raw sequence data; high scalability	May miss 3D structure-specific interactions

Challenges in AI Development

Challenge	Description	Impact
1. Data Availability & Quality	Lack of access to high-quality, diverse, and annotated datasets for training AI models. Much of the clinical and pharmaceutical data is proprietary or incomplete.	Results in biased, inaccurate, or non-generalizable models.
2. Data Privacy & Security	Use of sensitive health records and genetic information raises legal and ethical concerns regarding patient confidentiality.	Compliance with GDPR, HIPAA, etc., becomes complex and restrictive.
3. Regulatory Hurdles	Lack of standardized guidelines from regulatory bodies like FDA or EMA for AI-powered solutions.	Slows down deployment and market approval of AI systems in healthcare.

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4. Interpretability ("Black Box")	Deep learning models (e.g., neural networks) often lack transparency, making it hard to explain how decisions are made.	Reduces trust among clinicians, regulators, and patients.
5. Generalizability	AI models trained on specific datasets may not perform well in other populations or conditions.	Limits scalability and real-world clinical use.
6. Integration with Existing Systems	Difficulty integrating AI tools with Electronic Health Records (EHR), legacy systems, and hospital infrastructure.	Disrupts workflows and requires substantial IT changes.
7. High Computational Costs	Training advanced AI models (like AlphaFold or GANs) requires significant GPU/TPU power and cloud infrastructure.	Resource-intensive and expensive, especially for smaller institutions or developing nations.
8. Ethical Concerns	Risk of algorithmic bias, unequal access to AI tools, and automation displacing human roles.	Raises moral dilemmas and societal pushback.
9. Skill Gap	Shortage of interdisciplinary professionals skilled in both AI and life sciences (e.g., pharma, biology).	Slows research and implementation of AI solutions.
10. Validation & Benchmarking	Lack of universally accepted benchmarks for AI performance in different pharmaceutical stages (e.g., drug discovery vs clinical trials).	Makes model evaluation inconsistent and non-comparable.
11.Ethical AI Governance	Governance frameworks for responsible AI (transparency, accountability, inclusiveness) are still emerging.	Increases risk of misuse or unchecked consequences.

Limitations of Artificial Intelligence in Pharmacy

Limitation	Description	Impact
1. Limited Clinical Validation	Many AI models lack rigorous validation through clinical trials or real-world settings.	Reduces trust among healthcare professionals and hinders regulatory approval.
2. Data Dependency	AI systems rely on large, high-quality datasets (EHRs, trials, genomics), which may not always be available or standardized.	Leads to biased predictions and poor generalization across different populations.
3. Black Box Nature	Deep learning models often provide no clear reasoning behind their outputs.	Makes it difficult for clinicians to interpret or justify AI-driven decisions.
4. Regulatory Uncertainty	AI in pharmacy faces a lack of standardized regulatory pathways for approval and monitoring.	Delays in deployment and commercial adoption of AI tools.
5. Integration Challenges	Difficulty integrating AI with hospital systems, EHRs, and lab infrastructure.	Limits practical, real-time use in pharmacy operations.

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6. Incomplete Knowledge Representation	AI models cannot always represent complex biological systems, polypharmacy interactions, or rare diseases.	May miss out on crucial patient safety concerns or therapeutic insights.
7. Overfitting and Bias	AI may learn from noise or bias in training data (e.g., gender, ethnicity, geographic disparities).	Leads to unsafe, unequal, or inaccurate recommendations.
8. Cost of Implementation	High computational, licensing, and training costs.	Barrier for small-scale pharmacies, developing countries, and academic institutions.
9. Ethical and Legal Concerns	Patient data usage, informed consent, and liability for errors caused by AI remain unsettled.	Raises risks of misuse, litigation, and erosion of patient trust.
10. Lack of Human-AI Collaboration	Many AI systems are not designed to augment pharmacist decisions but to automate tasks entirely.	Reduces acceptability and can lead to resistance from healthcare providers.

CONCLUSION

In conclusion, AI is a game-changing foundation in the rapidly changing field of pharmaceutical research, intimately related to the abstract's concerns. AI is changing clinical diagnostics, patient-centered care, and the drug development process by combining cutting-edge technologies including generative models, deep learning, machine learning, and natural language processing. This study has demonstrated how AI's many classifications—based on capacity, functionality, and learning approach—allow for its wide range of applications in pharmacy, from telemedicine and customized medicine to molecular design and clinical trial optimization.

The effective use of AI-powered platforms such as DeepChem and AlphaFold2 is an example of how computational tools are enhancing safety and efficacy while cutting costs and timescales related to drug discovery. AI's significance in developing a more adaptable and effective healthcare system is highlighted by its ability to improve data analysis from electronic health records, forecast the course of diseases, and customize tailored treatments.

As AI develops further, its application in pharmacy holds potential for more innovation, better patient outcomes, and a move toward individualized, data-driven healthcare solutions. But achieving its full potential necessitates constant focus on moral issues, legal requirements, and multidisciplinary cooperation. In addition to becoming technologically sophisticated, the future of pharmacy will be more efficient, inclusive, and compassionate if AI is accepted as a scientific and strategic advantage. AI is not just helping the pharmacy industry in this new era; it is actively influencing it.

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