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IMPACT OF ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL INDUSTRY

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ABSTRACT

The pharmaceutical sector is experiencing significant advancements with the integration of artificial intelligence (AI). Many pharmaceutical companies are adopting this technology to enhance the drug discovery and development phases, which will facilitate various research-oriented projects related to novel drug delivery approaches. The speed at which AI operates can reduce the time lag between the development of a drug product and its commercialization. Additionally, AI is being utilized in clinical trials to generate and interpret data collected from patients. In this article, we will discuss the various roles of artificial intelligence in drug development, tablet manufacturing, the design of antibiotic peptides, and clinical research. This overview highlights the significant impact that artificial intelligence has on the pharmaceutical industry. One of the most important advantages of AI is its ability to reduce costs associated with drug development. This, in turn, enhances returns on investment and may lead to lower prices for end users. The present review article explores topics such as drug discovery, diagnosis, prediction of new treatments, the development of novel peptides from natural foods, treatment and management of rare diseases, drug adherence, and dosage challenges related to the adoption of artificial intelligence in the pharmaceutical industry.

KEYWORDS: Artificial intelligence and machine learning are transforming the pharmaceutical industry, particularly in drug discovery, manufacturing, and clinical trials.

Key concepts include ADME (Absorption, Distribution, Metabolism, and Excretion), AI software, applications of AI in the pharmaceutical sector, ANN (Artificial Neural Network), CT (Computed Tomography), DL (Deep Learning), and DNN (Deep Neural Network).

KEY MESSAGE

AI is transforming pharmaceutical research and development by streamlining drug discovery, improving clinical trial efficiency, and supporting personalized therapy.

INTRODUCTION

Artificial Intelligence (AI) is a branch of study that focuses on intelligent machine learning, particularly through computer programs that produce outcomes similar to human cognitive processes.[8] This process typically involves gathering data, creating effective methods for utilizing that data, deriving accurate or approximate conclusions, and making necessary modifications or adjustments.[9] AI is primarily used to analyze machine learning in order to mimic human cognitive functions.[8,9]

AI has significantly transformed the pharmaceutical industry, being applied across various fields of healthcare. Currently, many pharmaceutical companies face considerable challenges in drug discovery and development due to limited research resources and high costs. Consequently, AI technology is proving to be a valuable asset for efficient drug development. This technology represents a fusion of human intelligence and computer processing, serving as an advanced computer-aided technique that involves collecting information from multiple sources, establishing rules for handling this information, and generating possible outcomes to derive appropriate results and conclusions. Various statistical tools are employed in AI to enable computer software and processes to replicate human behavior. AI encompasses sub fields such as machine learning and deep learning, which simplify working with neural networks. The entire process of drug development, from identifying potential compounds to determining lead molecules and ultimately formulating drugs, including clinical trials, involves AI techniques. Therefore, AI is crucial for fostering innovation in the pharmaceutical sector and for ensuring the more accurate and rapid production of medicines.[2] Neural networks are a type of computational and mathematical model that analyze relationships within data without requiring prior knowledge from the user. While they do not provide specific predictions, they generate a range of possible outcomes that best align with the experimental data, thus meeting established criteria.

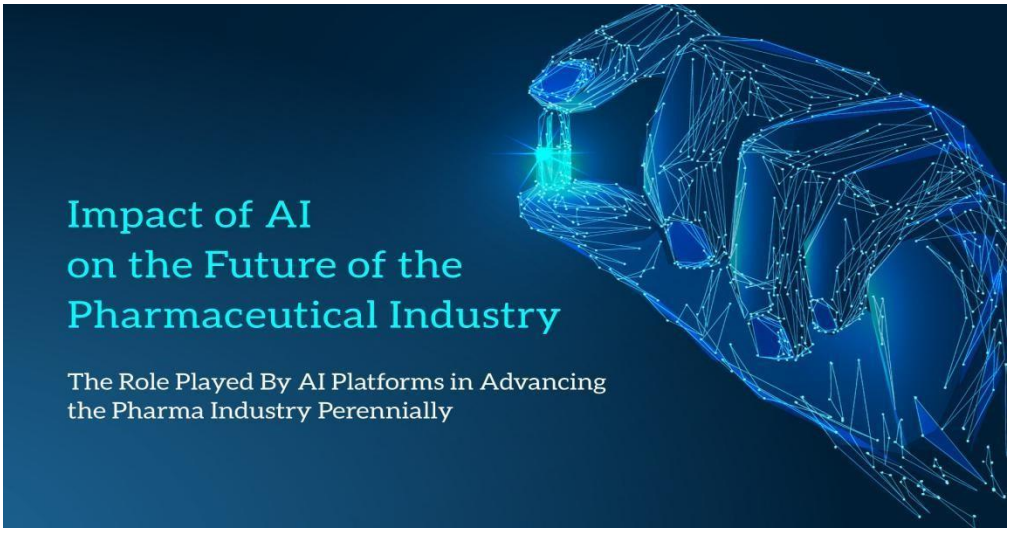


Figure 1: Impact of Artificial Intelligence In Pharmaceutical Industry.

Further, this technique is modified to develop Artificial Neural Networks (ANN) that is worthwhile in tackling problems related to pharmaceutical research, development and formulation.[3] The optimization process can be suitably conducted with another form of artificial intelligence technology called as fuzzy logic. It simplifies the complicated concepts and involves data mining and presenting the information in an easy format so that the user can directly interpret it, and devise actions accordingly by formulating rules that would serve as guidance for conducting the progress of work efficiently and developing future prospects.[1]

Classification of AI

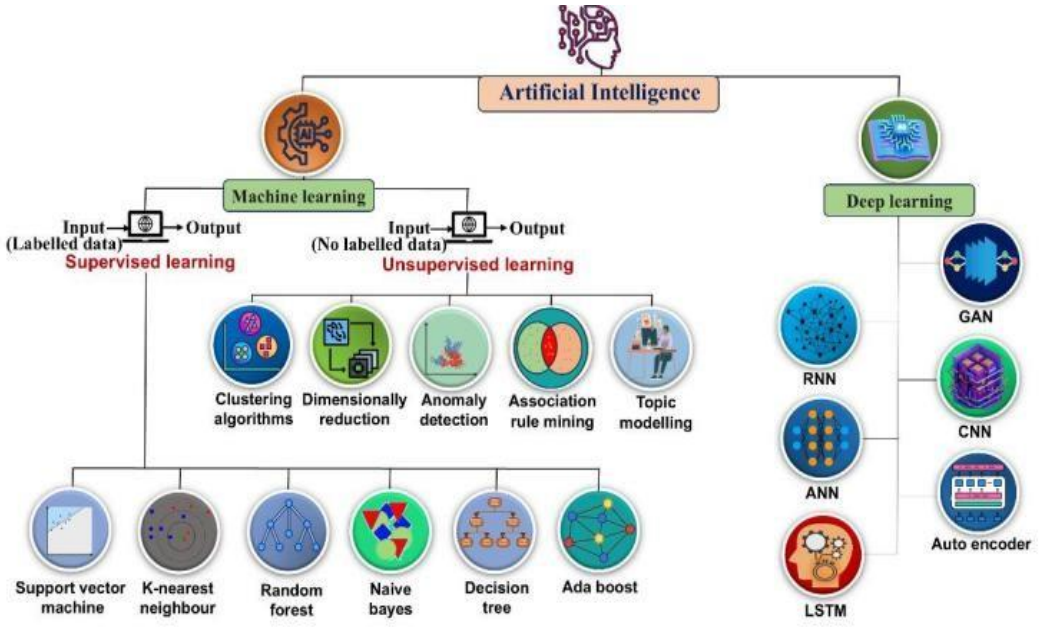


Figure 2: Classification of AI.

Historical Background

The Logic Theorist was created by Allen Newell and Herbert A. Simon. The first renowned conference on artificial intelligence took place at Dartmouth College in 1956.[4] The artificial intelligence market is expected to generate significantly more revenue between 2017 and 2022. Specifically, the market for natural language processing, which has applications such as text prediction and speech recognition, is projected to expand by 28.5% in 2017. In 2015, the global revenue from big data and business analytics amounted to $122 billion, and it is anticipated that this figure will exceed $200 billion by 2020.[5] Since the 1950s, the field of artificial intelligence has experienced a tumultuous history. The perception of AI as a mere dream shifted when IBM's Deep Blue computer defeated chess champion Garry Kasparov in 1997.

In 2011, IBM's new Watson supercomputer won a $1 million prize on the game show Jeopardy. Since then, Watson has expanded its applications into the healthcare and pharmaceutical industries, forming a partnership with Pfizer in 2016 to accelerate the development of new immuneoncology drugs. In December 2016, IBM and Pfizer unveiled IBM Watson, a cloud-based platform designed to help researchers discover connections across various data sets using dynamic visualization.[6] Scientists and engineers working on intelligent machines have made significant progress in enhancing the speed and memory capabilities of these devices, allowing them to outperform humans in many areas. However, the intellectual mechanisms of even the most advanced robots remain constrained by the limitations of what their designers can program. With the rise of big data, companies are leveraging artificial intelligence to provide more targeted solutions across various sectors, enabling them to analyze data in real time. The key milestones are summarized in Table 1.[7]

Table 1: Milestones in the Artificial Intelligence Process.

Years	Milestones
1943	Neurons can perform logical operations such as “and,” “or,” and “not” when connected in a network. This concept was demonstrated by Walter Pitts and Warren McCulloch.
1951	The first neural network that solved a real-world problem, known as SNARC (Stochastic Neural Analog Reinforcement Computer), was created by Marvin Minsky.
1956	At Dartmouth college conference the term “Artificial Intelligence” was coined.
1958	Perceptrons, which are neural networks that transmit information in one direction, were created by Frank Rosen blatt and serve as the foundation for today's AI advancements.
1969	Minsky advocated for the symbolic representation of problems in his book, "Perceptrons."

1974-1980	During this period interest on AI was dropped, which is called as "First AI Winter".
1986	The back propagation algorithm was developed by Geoffrey Hinton and is widely used in deep learning today.
1987-1993	This phase is called as "AI Winter"
1997	This year IBM Deep blue defeated the Garry Kasparov (Russian grandmaster).
2013	Google used British Technology to perform efficient research on photos.
2016	Google DeepMind's software, AlphaGo, defeated the Go champion Lee Sedol.

Types of Artificial Intelligence[10]

AI is wide ranging concept and can be classified into a number of ways. Based upon their caliber, AI system is classified as follows:

1) Weak intelligence or Artificial narrow intelligence (ANI)

This system is designed and trained to perform a narrow task, such as facial recognition, driving a car, playing chess, traffic signaling. E.g. Apple SIRI virtual personal assistance, tagging in social media.

2) Artificial General Intelligence (AGI) or Strong AI

It is also called as Human Level AI. It has the ability to simplify human intellectual abilities. Due to this, when it exposed to an unfamiliar task, it has the ability to find the solution. AGI can perform all the things as humans.

2) Artificial Super intelligence (ASI)

It is a brain power, which is more active than smart humans drawing, mathematics, space, etc. In each and every field from science to art, it ranges from the computer just little than the human to trillion times smarter than humans.

Tools of AI[12-13]

Robot Pharmacy

The objective of improving the safety of patients, UCSF Medical Center uses robotic technology for the preparation and tracking of medications. According to them, the technology has prepared 3,50,000 medication doses without any error. The robot has proved to be far better humans both in size as well as its ability to deliver accurate medications. The abilities of the robotic technology include preparations of oral as well as Injectables medicines which include chemotherapy drugs that are toxic. This has given freedom to the pharmacists and nurses of UCSF so that they can utilize their expertise by focusing on direct patient care and working with the physicians.

Figure 3: Robot Pharmacy.

MEDi Robot

MEDi stands for Medicine and Engineering Designing Intelligence. This pain management robot was developed as part of a project led by Tanya Beran, a professor of Community Health Sciences at the University of Calgary in Alberta. She was inspired to create MEDi after observing children who would scream during medical procedures in hospitals.[10] The robot is designed to build rapport with children and helps guide them through medical procedures. It teaches them how to breathe and cope with the experience. Although MEDi does not possess true thinking, planning, or reasoning abilities, it can be programmed to simulate aspects of artificial intelligence. Manufactured by Aldebaran Robotics, MEDi features built-in facial recognition technology and can respond to 20 different scenarios. The retail price of the robot is $9,000, but the cost can increase to between $15,000 and $30,000 when additional applications necessary for medical procedures are installed. Initially developed for pain management, the robot's applications have since expanded to include providing comfort during procedures, assisting with physical rehabilitation, and supporting fundraising Efforts.

Figure 4: MEDi Robot.

Figure 5: MEDi Interacting with Child.

Erica Robot

Erica is a new care robot that has been developed in Japan by Hiroshi Ishiguro, a professor at Osaka University. The creation of Erica involved collaboration with the Japan Science and Technology Agency, Kyoto University, and the Advanced Telecommunications Research Institute International (ATR). While the robot cannot walk independently, it possesses the ability to understand and respond to questions with human-like facial expressions. Ishiguro describes Erica as the "most beautiful and intelligent" android, as he based her features on an average derived from 30 beautiful women, carefully designing aspects such as the nose and eyes.

Figure 6: Erica – The Humanoid Robot.

Tug Robot

Aethon TUG robots are designed to autonomously navigate through hospitals and deliver medications, meals, specimens, and materials. They can also carry heavy loads such as linen and trash. The robots have two configurations: fixed carts and a secured exchange base platform. The fixed carts are specifically used for delivering medications, sensitive materials, and laboratory specimens, while the exchange platform is employed to transport items that can be loaded onto different racks. The TUG robots can deliver various types of carts or racks, making them a highly flexible and valuable resource.

Figure 7: TUG Robot Handling Pills.

Berg

Berg is a Boston-based biotechnology company that is a key player in utilizing AI across its various processes. The company has developed an AI-driven platform for drug discovery that features a large database of patients. This database is used to identify and validate biomarkers associated with diseases and to determine appropriate therapies based on the data collected. Berg's mission is to accelerate the drug discovery process and reduce costs by leveraging AI, which eliminates the guesswork typically involved in drug development. The steps followed by Berg include procuring sequencing data from human tissue samples, gathering information on metabolites and protein formation, and applying AI algorithms to accurately identify the underlying causes of diseases.

Various Role of AI in Pharmaceutical Industries

1. Role of Artificial Intelligence in Drug Development

Due to the expanding chemical space, the gap between drug discovery and development is increasing daily, making the search for novel drug molecules more tedious and challenging. Techniques grounded in artificial intelligence offer significant advantages across various critical phases of drug development, such as identifying and validating drug targets, modeling drug compounds, and enhancing their drug-like properties. AI also plays a vital role in designing clinical trials for patients, thus optimizing decision-making strategies. One notable application of AI is "Open Targets," a strategic program that investigates the relationship between drug targets and diseases, as well as the connections between genes and diseases. This program helps identify targets associated with specific diseases or the diseases related to particular targets.[4] Drug-like molecules must adhere to Lipinski's Rule of Five. With this in mind, a novel neural network technique known as 3N-MCTS (Monte Carlo Tree Search), developed by Seglar et al., has an advantage over traditional computer-aided retrosynthesis systems. This technique allows for the rapid development of various synthetic routes while reducing the number of steps involved.

Another AI approach, called SPIDER, is utilized to determine the role of natural products in drug discovery. It was specifically designed to predict the targets of drug molecules, such as β-Lapachone, demonstrating that reversible and allosteric inhibition of 5-Lipoxygenase is caused by this compound. For assessing the toxicity of unknown compounds, an advanced technique known as Read Across Structure Activity Relationship (RASAR) is employed. This tool is designed to create and identify connections between molecular structures and properties that can lead to toxicity, using databases available for chemicals.[4] The Deep Neural Network (DNN) is a system composed of artificially connected neurons that interact to perform various data transformations. It establishes criteria for classifying drugs into their respective therapeutic classes based on pharmacological and toxicological data. Networks such as Generative Adversarial Networks (GANs) serve as a foundation for developing next-generation AI techniques. Artificial Intelligence encompasses an important facet known as Machine Learning (ML), which relies on statistical attributes. Machine learning can be classified into three sections:

i. Supervised Learning

This approach is associated with developing predictive models using regression and classification methods. These models generate predictions based on input and output data.

The output data includes diagnostic methods for disease classification and efficacy predictions for drugs, as well as absorption, distribution, metabolism, and excretion (ADME) predictions categorized under regression analysis. Therefore, both of these subgroups provide extensive insights.[16]

ii. Unsupervised Learning

This method focuses exclusively on input data. Interpretations are drawn by clustering and grouping the data through feature extraction pathways. This type of learning can yield output data related to disease categories in the clustering subgroup, while the feature extraction subgroup contains information regarding the origin of targets for those diseases.[16]

iii. Reinforcement Learning

The primary function of this approach is to make decisions based on the environment and execute actions to achieve optimal performance. The outputs from this type of machine learning include drug design through a de novo approach, which falls under decision-making, and experimental drug design, which falls under execution. Both can be achieved through modeling techniques and the application of quantum chemistry.[16]

Furthermore, deep learning can be employed to identify genetic markers and various novel drug molecules. By applying artificial intelligence, we can address several shortcomings in pharmaceutical product development. This approach may also reduce the number of drugs failing in clinical trials, thereby accelerating the drug design and development process in a cost-effective manner.[16]

1.1 Drug development process

The development of drugs involves a series of systematic steps. This process begins with various techniques, such as High Throughput Screening (HTS) and computational modeling, which help generate valuable results. It consists of two alternating cycles known as the inductive and deductive cycles. These cycles work together to identify heat and lead compounds that meet the desired specifications. Errors in this process can be minimized through automation.[15] In the drug development process, novel compounds that exhibit the desired biological activity are selected and identified. This biological activity is assessed through interaction studies conducted with specific enzymes or organisms. The initial compound that demonstrates biological activity in response to a given target is referred to as a "hit" molecule. Libraries of different chemical compounds are screened to identify these hit

molecules. Additionally, computer simulations and the screening of various isolated natural products, such as those from bacteria, plants, and fungi, are employed to discover potential hit molecules.

The next step in drug development is lead identification. A lead molecule possesses the necessary properties to be advanced into the development of a drug for the targeted disease. Cell-based screening assays and animal models are used to assess the safety and efficacy of the generated hit series. After identifying a lead compound, structural modifications are carried out to alter its chemical properties, aiming to produce a compound with minimal toxicity and optimal therapeutic effects.[15] The lead generation phase involves modifying hit molecules to enhance their selectivity and affinity for the desired target, improve their biological activity, and reduce side effects, ultimately leading to the development of a safe and effective drug. Following this, hit expansion is performed to produce analogs— chemical compounds derived from hit molecules. These analogs are then combined through various reactions orchestrated by medicinal chemists, creating "building blocks," which are compounds containing essential functional groups for interaction with the target's active site. The active site is a specific area on the target that allows for the binding of drug molecules through various interactions, which can be described by the "lock and key" model.

Artificial intelligence (AI) can be effectively utilized for several purposes in drug development, including

- Identifying molecular targets and predicting the underlying mechanisms of drug-target interactions.
- Determining hit or lead compounds.
- Synthesizing compounds with drug-like properties.
- Repurposing existing drugs.
- Selecting appropriate populations for clinical trials.
- Studying and determining the modes of action of drugs. □□Designing polypharmacology agents.

2. Modulation of size distribution in granules by Artificial Intelligence

Computational Intelligence is being utilized to develop milling procedures that produce effective particle size distributions. The dry granulation method is the most commonly used technique for creating solid dosage forms. This method consists of two steps: first, the compaction of powder between two rolls rotating in opposite directions to create a ribbon;

and second, the milling process, where the crushing of these ribbons leads to the formation of granules. Particle size is a critical feature in pharmaceutical drug development. To determine and modulate it, various artificial intelligence technologies are being developed. This approach is also used to study different factors and properties of drugs that affect particle size. Important relationships are being identified, such as how material properties, milling parameters, and current conditions influence granule size distribution. Additionally, the change in granule size distribution resulting from roller compaction can be assessed using artificial intelligence systems that establish relationships between roller compaction parameters and their effects on granule size.[18,19]

Multiple linear regression is one computational method used to describe the impact of various independent factors on dependent variables. Artificial Neural Networks (ANNs) are employed to select the most relevant parameters for modeling granule size based on layered criteria. A typical ANN consists of three types of layers: the input layer, the hidden layer, and the output layer. These layers contain interconnected neurons through which signals travel from the input layer to the output layer via the hidden layers. In this model, a range is selected for each layer, and linear scaling is maintained within that range. Genetic Programming (GP) is another model based on Darwin's theory of evolution, which emphasizes the survival of the fittest. In this context, individuals that do not adapt or survive in the prevailing conditions are eliminated. Thus, GP selects and breeds those individuals that can adapt and demonstrate their fitness to the environment.[18]

3. Role of Artificial Intelligence in clinical Research

It has been observed that a significant number of drugs fail during clinical trials, and the percentage of drugs that successfully enter the market is declining. While some drug products may pass clinical trials, various issues can arise when they are introduced to the market. Consequently, there is a need for a digital platform designed to address these challenges. Although artificial intelligence (AI) has numerous applications, its use in clinical research remains largely theoretical due to a lack of scientific evidence. Nonetheless, AI plays a crucial role in clinical research and has a significant impact on several key aspects.[17]

- Success or failure rate of drug product.
- Reduction in the cost of product development in terms of absolute values.
- Reduction of time taken by the drug product to enter the market. Decrease in the number of product recalls.

Artificial Intelligence also focuses on the following three major objectives of clinical research

- Signals which are predictive and affect the disease pathology.
- The different steps and methods used for intervention.
- The effect of time on patient's condition and the way in which it defines the quality of life.

4. AI for Drug Discovery

AI has revolutionized drug research and discovery in numerous ways. Some of the key contributions of AI in this domain include the following:

Target Identification

AI systems can analyze a variety of data types, including genetic, proteomic, and clinical data, to identify potential therapeutic targets. By uncovering disease-associated targets and molecular pathways, AI aids in designing medications that can modify biological processes.

Virtual Screening

AI enables the efficient screening of extensive chemical libraries to identify drug candidates with a high likelihood of binding to specific targets. By simulating chemical interactions and predicting binding affinities, AI helps researchers prioritize and select compounds for experimental testing, thereby saving time and resources.

Structure-Activity Relationship (SAR) Modeling

AI models can establish connections between the chemical structures of compounds and their biological activities. This allows researchers to optimize drug candidates by designing molecules with desirable features, such as high potency, selectivity, and favorable pharmacokinetic profiles.

De Novo Drug Design

Using reinforcement learning and generative models, AI algorithms can propose novel, drug-like chemical structures. By learning from chemical libraries and experimental data, AI expands the chemical space and supports the development of innovative drug candidates.

Optimization of Drug Candidates

AI algorithms can analyze and optimize drug candidates by considering various factors, including efficacy, safety, and pharmacokinetics. This helps researchers fine-tune therapeutic molecules to enhance their effectiveness while minimizing potential side effects.

Drug Repurposing

AI techniques can examine large-scale biomedical data to identify existing drugs that may have therapeutic potential for different diseases. By repurposing approved drugs for new indications, AI accelerates the drug discovery process and reduces costs. **Toxicity Prediction** AI systems can predict drug toxicity by analyzing the chemical structures and characteristics of compounds. Machine learning algorithms trained on toxicology databases can anticipate harmful effects or identify hazardous structural properties. This helps researchers prioritize safer chemicals and mitigate potential adverse responses in clinical trials.

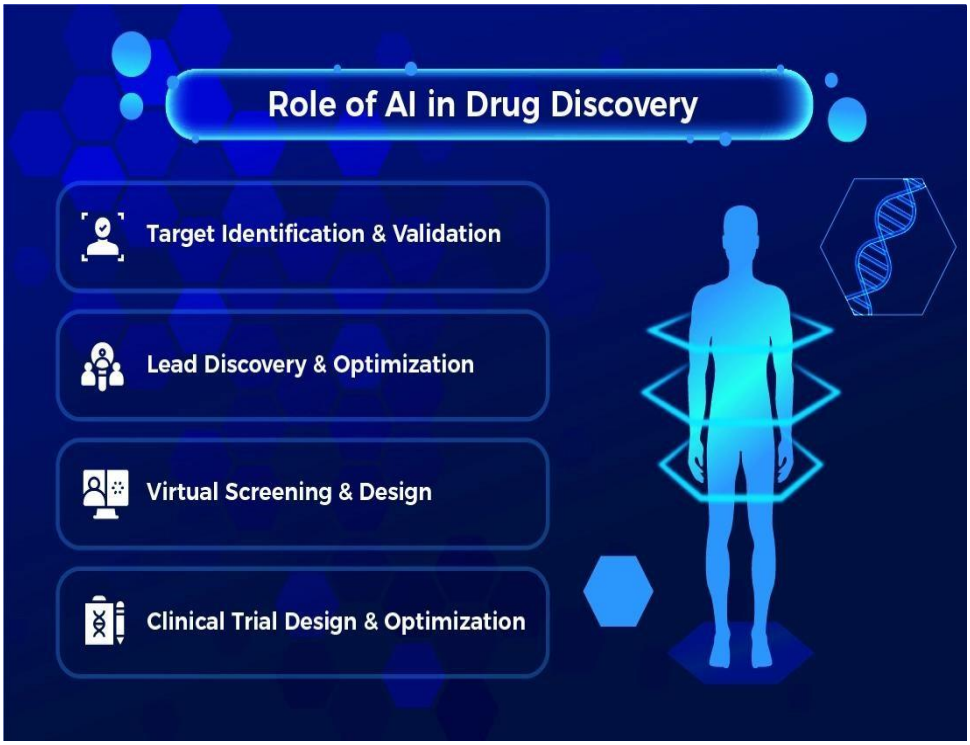


Figure 8: Role of AI in Drug Discovery.

AI-driven approaches in drug research and development have the potential to streamline and accelerate the identification, optimization, and design of novel therapeutic candidates, ultimately leading to more efficient and effective medications.[21]

One example of this is in silico target fishing(TF) technology, which is used in pharmaceuticals for predicting biological targets based on chemical structures. This information is derived from chemical databases that are biologically annotated. In addition to TF, various other methods, such as data mining and the docking of chemical structures, are employed to explore mechanisms of action and gather target class information needed for effective planning. The target fishing technique has become essential in drug discovery by leveraging machine learning and cheminformatics tools. These tools provide detailed insights into the analysis of complex structures and facilitate the design of novel drug ingredients for treating challenging diseases. Traditional drug discovery methods carried out by various industries can be quite costly, as they involve multiple intricate processes, including the identification and selection of target proteins and an in-depth understanding of the mechanisms of action for small molecules. To expedite this process, TF has been applied, significantly reducing the overall experimental costs associated with drug development.

Reference molecules are utilized to predict ligand-target interactions using 3D descriptors. This technique has successfully identified the high binding affinity of diethylstilbestrol. Additionally, the TF technique is extensively used to study the phytopharmacology of drugs and conduct monthly similarity assessments. Functioning as a computational and proteomics-based method, TF ranks data points based on data fusion similarity alongside drug targets. It is also employed to predict potential toxicities in the ligandbased approach used for drug discovery. Several critical aspects essential to drug development and discovery, such as novel target identification, selection, prediction of phytopharmacological profiles, and potential adverse effects associated with new therapeutic indications, are effectively explored using TF. Specifically, bioactive compound similarity is utilized for target identification related to unrecognized compounds. Successful drugs characterized by this method include loperamide, emetine, and methadone, with identified targets such as muscarinic, adrenergic, and neurokinin receptors.[22,23–24]

Table 2: Popular AI model tools used for drug discovery.

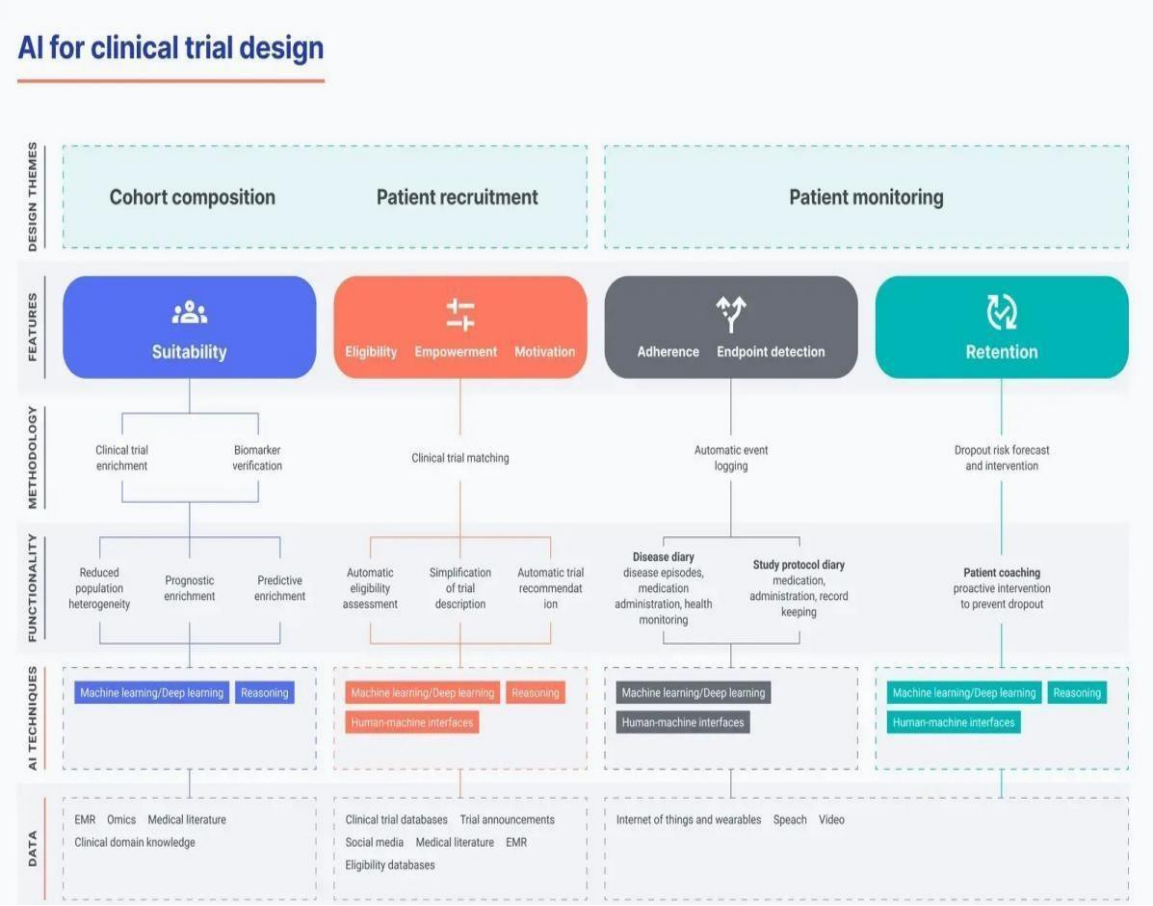
AI Model Tools	Summary
DeepChem	An open-source library that provides a wide range of tools and models for drug discovery, including deep learning models for molecular property prediction, virtual screening, and generative chemistry.
RDKit	A widely used open-source chem-informatics library that offers various functionalities for molecule handling, substructure searching, and descriptor calculation. It can be integrated with machine learning frameworks for drug

	discovery applications
ChemBERTa	A language model specifically designed for drug discovery tasks. It is based on the Transformer architecture and is pretrained on a large corpus of the chemical and biomedical literature, allowing it to generate molecular structures, predict properties, and assist in lead optimization.
GraphConv	A deep learning model architecture that operates on molecular graphs. It has been successful in predicting molecular properties, such as bioactivity and toxicity, by leveraging the structural information encoded in the graph representation of molecules.
AutoDock Vina	A popular docking software that uses machine learning techniques to predict the binding affinity between small molecules and protein targets. It can assist in virtual screening and lead optimization for drug discovery.
SMILE Transformer	A deep learning model that takes Simplified Molecular Input Line Entry System (SMILES) strings as input and generates molecular structures. It can be used for de novo drug design and lead optimization.
Schrödinger Suite	A comprehensive software package for drug discovery that incorporates various AIdriven tools. It includes modules for molecular modeling, virtual screening, ligandbased and structure-based drug design, and predictive modeling.
IBM RXN for Chemistry	An AI model designed to predict chemical reactions. It utilizes deep learning algorithms and large reaction datasets to generate potential reaction outcomes, aiding in the discovery of new synthetic routes and compound synthesis.
scape-DB	scape-DB (Extraction of Chemical and Physical Properties from the LiteratureDrugBank) is a database that combines natural language processing and machine learning to extract chemical and biological data from the scientific literature. It provides valuable information for drug discovery research.
GENTRL (Generative Tensorial Reinforcement Learning)	A deep learning model that combines reinforcement learning with generativ chemistry to design novel molecules with desired properties. It has been used for de novo drug design and optimization.

5. AI in Clinical Trial Design

Clinical trials aim to establish the safety and efficacy of drug products in humans for specific disease conditions. These trials typically require 6 to 7 years and a substantial financial investment. Unfortunately, only one out of every ten molecules that enter these trials receives successful clearance, resulting in significant losses for the industry. Failures can arise from factors such as inappropriate patient selection, insufficient technical resources, and inadequate infrastructure. However, with the extensive digital medical data available, these failures can be reduced by implementing artificial intelligence (AI).[26] Patient enrollment accounts for one-third of the clinical trial timeline. The success of a clinical trial heavily depends on recruiting suitable patients, as poor selection contributes to approximately 86% of trial failures.[27] AI can aid in identifying specific patient populations for recruitment in Phase II and III of clinical trials by analyzing patient-specific genome-exposome profiles.

This approach assists in the early prediction of potential drug targets for the selected patients.[28,29] Additionally, AI applications, such as predictive machine learning and reasoning techniques, can facilitate the preclinical discovery of molecules, helping to identify lead compounds likely to succeed in clinical trials based on the selected patient population.[26] Patient dropout accounts for 30% of clinical trial failures, necessitating additional recruitment efforts to complete the trial, which wastes time and resources. This issue can be mitigated through close monitoring of patients and supporting their adherence to the trial protocols. For instance, Ai Cure developed a mobile application that monitored medication intake for patients with schizophrenia during a Phase II trial, resulting in a 25% increase in patient adherence and ensuring the successful completion of the trial.[28]



6. AI in designing Drug Molecules

Prediction of Target Protein Structure When developing a drug molecule, it is crucial to identify the correct target for successful treatment. Numerous proteins are involved in disease development, and in some cases, they are over-expressed. Therefore, predicting the structure of the target protein is vital for selective targeting of the disease and for designing effective drug molecules. Artificial intelligence (AI) can aid in structure-based drug discovery by

predicting the 3D structure of proteins. This prediction aligns with the chemical environment of the target protein site, enabling the assessment of a compound's effect on the target, as well as safety considerations before synthesis or production.[29] One AI tool, Alpha Fold, which relies on deep neural networks (DNNs), analyzes the distances between adjacent amino acids and the corresponding angles of peptide bonds to predict 3D protein structures. It has demonstrated impressive results, accurately predicting 25 out of 43 structures. In a study by AlQurashi, a recurrent neural network (RNN) was utilized to predict protein structure through three stages: computation, geometry, and assessment, termed a recurrent geometric network (RGN).

In this approach, the primary protein sequence was encoded, and the torsional angles for a given residue, along with a partially completed backbone from the geometric unit, were considered as input; this produced a new backbone as output. The final unit generated the 3D structure as the output. The accuracy of the predictions was assessed using the distance-based root mean square deviation (dRMSD) metric, with parameters optimized to minimize dRMSD between experimental and predicted structures. AlQurashi predicted that his AI method would be quicker than AlphaFold for predicting protein structures. However, AlphaFold is expected to have greater accuracy when predicting structures with sequences similar to reference structures.[30] A study also predicted the 2D structure of a protein using MATLAB, assisted by a nonlinear three-layered neural network (NN) toolbox based on feedforward supervised learning and back-propagation error algorithms. MATLAB was employed to train input and output data sets, and the NNs served as learning algorithms and performance evaluators. The accuracy in predicting the 2D structure was found to be 62.72%.[32]

Predicting Drug–Protein Interactions

Drug–protein interactions are crucial for the success of therapeutic interventions. Understanding how a drug interacts with a receptor or protein is essential for assessing its efficacy and effectiveness. Accurate predictions of these interactions allow for drug repurposing and help avoid poly-pharmacology.[29] Various AI methods have been effective in predicting ligand–protein interactions, thereby enhancing therapeutic efficacy.[29,33] For instance, Wang et al. reported a model using the support vector machine (SVM) approach, trained on 15,000 protein–ligand interactions, which focused on the primary protein sequences and structural characteristics of small molecules. This model successfully

identified nine new compounds and their interactions with four key targets.[34] Yu et al. utilized two random forest (RF) models to predict drug–protein interactions by integrating pharmacological and chemical data, validating their findings against known platforms like SVM, achieving high sensitivity and specificity. These models are capable of predicting drug–target associations that can be further extended to target–disease and target–target associations, accelerating the drug discovery process.[35] Xiao et al. adopted the Synthetic Minority Over-Sampling Technique and Neighborhood Cleaning Rule to optimize data for the subsequent development of iDrugTarget, which combines four subpredictors: iDrug-GPCR, iDrug-Chl, iDrug-Enz, and iDrug-NR. These subpredictors identify interactions between drugs and G-protein-coupled receptors (GPCRs), ion channels, enzymes, and nuclear receptors (NR), respectively. When compared with existing predictors through target-jackknife tests, iDrugTarget outperformed its counterparts in terms of both prediction accuracy and consistency.[36]

The capability of AI to predict drug-target interactions has been effectively utilized in repurposing existing drugs while minimizing the risk of polypharmacology. Repurposing a drug allows it to qualify directly for Phase II clinical trials.[28] This process is cost-effective, as relaunching an existing drug costs approximately US$8.4 million, in contrast to the US$41.3 million required to launch a new drug entity.[37] One approach used in this context is the "Guilt by Association" method, which helps forecast novel associations between drugs and diseases. This approach can be either knowledge-based or computationally driven. In computational networks, machine learning (ML) techniques are commonly employed, utilizing methods such as support vector machines (SVM), neural networks (NN), logistic regression, and deep learning (DL). Logistic regression platforms, including PREDICT, SPACE, and other ML approaches, evaluate factors such as drug-drug and disease-disease similarities, the likeness of target molecules, chemical structures, and gene expression profiles to effectively repurpose drugs.[39] Additionally, a cellular network-based deep learning technology known as deepDTnet has been explored to predict the therapeutic applications of topotecan, which is currently used as a topoisomerase inhibitor.[42] This drug may also be repurposed for treating multiple sclerosis by inhibiting the human retinoic acid receptor-related orphan receptor-gamma t (ROR-γt). This platform is presently under a provisional US patent. Self-organizing maps (SOMs), categorized under unsupervised machine learning, are also employed in drug repurposing. They use a ligand-based approach to search for novel off-targets among a set of drug molecules, training the system on a

specific number of compounds with known biological activities for subsequent analysis of different compounds. In a recent study, deep neural networks (DNN) were used to repurpose existing drugs with established activity against SARS-CoV, HIV, and influenza virus, as well as drugs that act as 3C-like protease inhibitors.[42] The research considered extended connectivity fingerprints (ECFP), functional-class fingerprints (FCFPs), and the octanol-water partition coefficient (ALogP_count) to train the AI platform. The findings indicated that 13 of the screened drugs could progress toward further development based on their cytotoxicity and ability to inhibit viral activity.[42]

Drug-protein interactions can be used to predict the likelihood of polypharmacology, which refers to a drug molecule's tendency to interact with multiple receptors, potentially leading to off-target adverse effects.[43] Artificial intelligence (AI) can assist in designing new molecules based on the principles of polypharmacology, contributing to the development of safer drug molecules.[44] AI platforms, such as SOM, combined with extensive databases, can link various compounds to multiple targets and off-targets. Bayesian classifiers and Similarity Ensemble Approach (SEA) algorithms are valuable tools for establishing connections between the pharmacological profiles of drugs and their potential targets.[41] Li et al. demonstrated the use of KinomeX, an AI-based online tool utilizing deep neural networks (DNNs) to detect the polypharmacology of kinases based on their chemical structures. This platform is trained on approximately 14,000 bioactivity data points derived from over 300 kinases. It has practical applications in studying the overall selectivity of a drug towards the kinase family and specific subfamilies, thus aiding in the design of novel chemical modifiers. In their study, they used NVP-BHG712 as a model compound to predict both its primary targets and off-targets with reasonable accuracy.[45]

Another noteworthy example is Cyclica’s Ligand Express, a cloud-based proteome screening AI platform that identifies receptors capable of interacting with specific small molecules. This tool helps in understanding both on- and off-target interactions, which can reveal possible adverse effects of drugs. In recent years, the de novo drug design approach has gained popularity for creating drug molecules. Traditional de novo design methods are being supplanted by advanced deep learning (DL) techniques, which address the shortcomings of complex synthesis routes and the difficulty in predicting the bioactivity of novel molecules.[47] Computer-aided synthesis planning can propose millions of potential structures and various synthesis routes.[48] Grzybowski et al. developed the Chematica program[49], now

known as Synthia, which encodes a set of rules into the system to suggest possible synthesis routes for eight medically important targets. This program has proven efficient in improving yields and reducing costs, and it can also provide alternative synthesis strategies for patented products, facilitating the synthesis of compounds that have not been produced before. Similarly, DNNs focusing on organic chemistry rules and retrosynthesis, supplemented by Monte Carlo tree searches and symbolic AI, significantly enhance reaction predictions, leading to quicker drug discovery and design processes compared to traditional methods.[50,51] Coley et al. created a framework using a rigid forward reaction template applied to a set of reactants to yield chemically feasible products at high reaction rates. Machine learning (ML) was used to identify the dominant product based on a score determined by neural networks.

Additionally[52], Putin et al. explored a DNN architecture known as thereinforced adversarial neural computer (RANC), which employs reinforcement learning (RL) for the de novo design of small organic molecules. This platform was trained using molecules represented as SMILES strings and generated new molecules with specific chemical descriptors, including molecular weight (MW), logP, and topological polar surface area (TPSA).[53] RANC demonstrated superior performance in generating unique structures compared to another platform, ORGANIC, while maintaining structural integrity. Furthermore, recurrent neural networks (RNNs) based on long short-term memory (LSTM) were applied to molecules obtained from the ChEMBL database and encoded as SMILES strings. This approach successfully generated a diverse library of molecules for virtual screening (VS) and was extended to produce novel molecules targeting specific areas, such as the 5-HT2A receptor, Staphylococcus aureus, and Plasmodium falciparum.[54]

Popova et al. developed the Reinforcement Learning for Structural Evolution strategy for de novo drug synthesis, which utilizes generative and predictive deep neural networks (DNNs) to create new compounds. In this approach, the generative model produces unique molecules based on SMILE strings and uses a stack memory, while the predictive models forecast the properties of the developed compounds. Merk et al. also utilized a generative AI model to design retinoid X and PPAR agonist molecules with specific therapeutic effects, without the need for complex rules. They successfully designed five molecules, four of which demonstrated strong modulatory activity in cell assays, highlighting the effectiveness of generative AI in synthesizing new molecules. The integration of AI in the de novo design of molecules offers significant benefits to the pharmaceutical industry. It facilitates online

learning and allows for the simultaneous optimization of previously learned data, as well as suggesting potential synthesis routes. This leads to faster lead design and development.[54,57]

7. Al in pharmacovigilance

AI systems integrate various data sources, such as electronic health records (EHRs), social media, and patient forums, to identify adverse drug reactions (ADRs). This comprehensive approach captures patient experiences that are often overlooked by traditional methods, thereby enhancing drug safety monitoring and post-market surveillance.[58] Unstructured data, including social media comments and patient discussions in forums, is processed using Natural Language Processing (NLP) to analyze this information. AI identifies different patterns and signals related to ADRs that are typically missed by conventional methods.[59] Pattern recognition employs machine learning algorithms designed to detect patterns in large datasets. With the aid of AI, real-time monitoring enables the immediate detection of ADRs as they occur, facilitating quick responses to potential safety issues. The effectiveness of ADR detection using AI largely depends on the quality and quantity of the data it processesas shown in figure 2.[60] Pharmacovigilance is being revolutionized by various AI-powered tools that enhance the detection of adverse events and drug safety monitoring. For example, AstraZeneca uses an AI-based system to detect adverse events and support regulatory compliance; however, this system requires skilled personnel and may overlook rare events. IBM Watson for Drug Safety utilizes machine learning and NLP to analyze both structured and unstructured data, thereby improving decision-making. Adverse Health Analytics employs SignalMine for efficient monitoring of adverse events and risk assessment, while Oracle's Argus Safety automates signal detection and adverse event reporting.[61]

AI And FDA approval and post-marketing surveillance

NLP can be utilized to analyse scientific literature for identifying and reporting adverse effects like drug toxicity or resistance. Additionally, NLPbased sentiment analysis techniques can assist in recommending drugsas shown in figure 9. Machine learning systems can also predict potential product sales, allowing pharmaceutical companies to better allocate and optimize their business resources.[62]

□□CASE STUDY

In our overview of AI software in drug discovery, let's nowexplorereal-world applications through case studies that demonstrate the significant impact these technologies have had in the field. One notable case study is "Benevolent AI – Using AI to Disrupt the Traditional

Drug Discovery Process." This UK-based company utilizes its AI platform, the Bioscience Machine Brain (BMB), to transform the drug discovery process. Benevolent AI has managed to reduce the time required for earlyphase and preclinical testing from 3 to 6 years down to just 1 to 2 years, while also lowering costs by 60%. This innovative platform has quickly identified promising compounds for ALS, which are now in clinical trials. The study highlights Benevolent AI's potential to disrupt the pharmaceutical industry, especially as health-tech startups and pharmaceutical giants increasingly adopt AI technologies. As a result, significant advancements in the treatment of severe diseases are becoming more attainable.

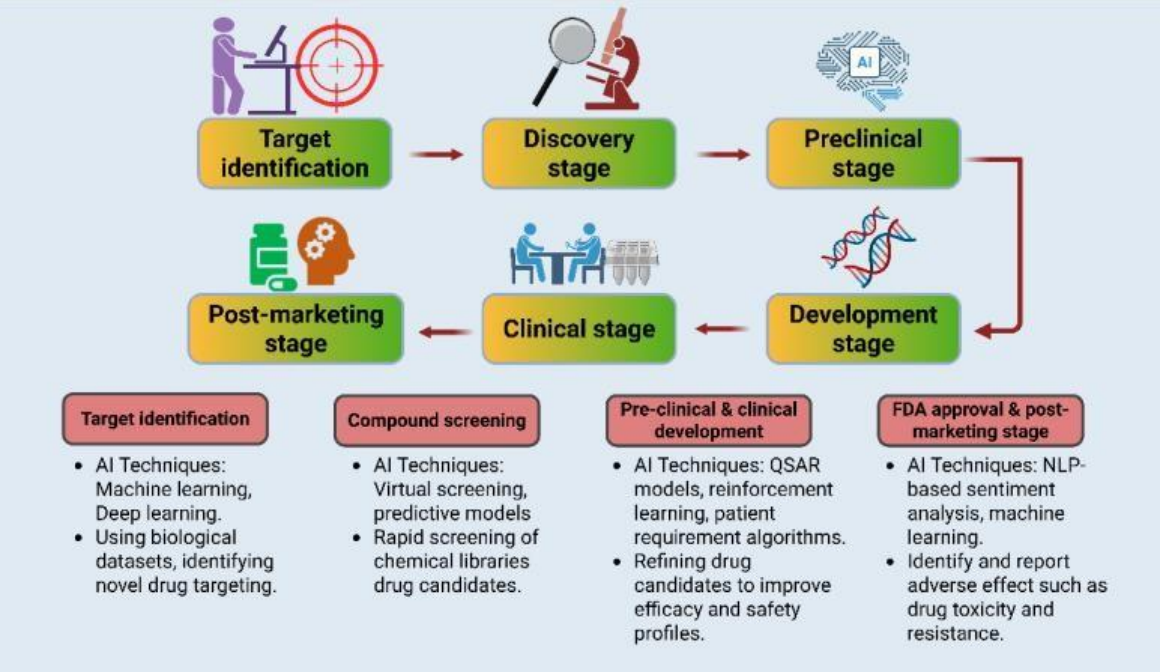


Figure 9: AI in drug Discovery.

AI in quality control and quality assurance

Pharmaceutical quality control is undergoing a significant transformation due to artificial intelligence (AI), particularly in drug release prediction, as illustrated in Figure 10. Factors such as tablet geometry, drug loading, and compaction pressure influence drug release, which is assessed through in vitro and in vivo studies and is critical in the development of new products.[63] Conducting drug release research using traditional spectrophotometric and analytical techniques can be complex and time-consuming. However, AI techniques like artificial neural networks (ANN), support vector machines (SVM), and regression analysis now enable accurate predictions of dissolution profiles, drug release rates, and disintegration times.[63]

Incorporating AI and machine learning (ML) into Six Sigma documentation significantly enhances quality control. ML algorithms employ predictive analytics to analyze historical data, identify patterns, and anticipate potential quality issues, facilitating proactive interventions and reducing risks. Additionally, predictive maintenance helps foresee equipment failures by monitoring usage trends.[64] One of the leading pharmaceutical companies utilized ML models and AI-driven data collection to automate its documentation process, track essential quality metrics, and detect possible deviations at an early stage. AI-driven validation checks ensured data integrity and compliance. This approach fostered operational excellence and continuous improvement by enhancing efficiency, decreasing compliance risks, and strengthening overall quality assurance.[64]

The applications of AI in the pharmaceutical and healthcare sectorsvast and include areas such as drug discovery and development, pharmaceutical manufacturing, insulin development, nanobots, personalized medicine, clinical applications, quality control and assurance, pharmacovigilance, gene biomarkers, and drug repurposing, as shown in Figure 10.

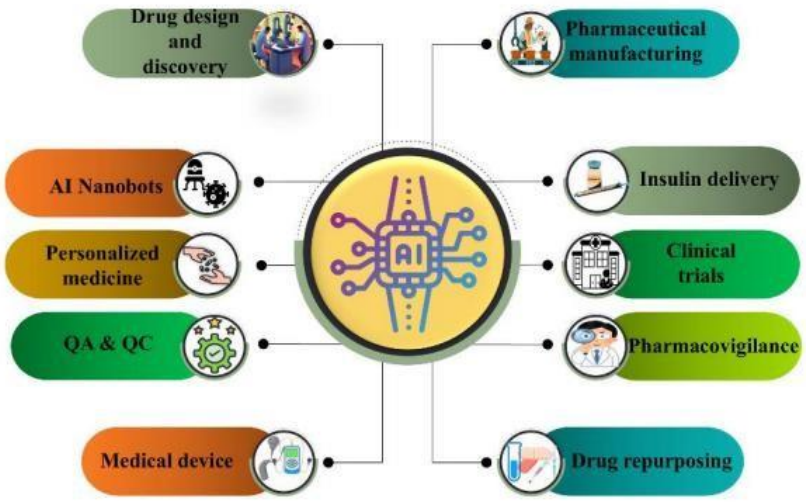


Figure 10: Application of AI in different pharmaceutical domain.

8. CONCLUSION

In summary, the implementation of AI in pharmacy has the potential to completely transform the profession and provide significant benefits for both patients and pharmacists. It could enhance medication management, improve patient outcomes, facilitate drug discovery, and expedite the development of new medications by increasing accuracy and safety in

medication administration. Additionally, AI advancements may help reduce healthcare costs. Although there are challenges to adopting AI in the pharmacy sector, its potential to revolutionize this field is evident. AI has already impacted various areas within the pharmaceutical sector, including drug discovery, development, manufacturing, and quality assurance.

The most notable changes have involved speeding up processes, increasing efficiency, and improving outcomes due to the vast amount of data that can now be processed, accelerated, and analyzed. AI has strengthened our ability to recognize patterns, make data-driven assumptions, and enhance decisionmaking. Moreover, it has contributed to the personalization of individual therapies. AI has also played a role in ensuring regulatory compliance, securing data, and addressing intellectual property concerns, while continuing to enhance efforts in these areas. I believe that AI will significantly impact the advancement of the pharmaceutical industry, fostering innovation and development while improving patient outcomes in the future. Within the next decade, it is likely to shape the overall future of healthcare as well.

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