



## INDO AMERICAN JOURNAL OF PHARMACEUTICAL RESEARCH



### ARTIFICIAL INTELLIGENCE: AN EVOLVING TOOL IN PHARMACEUTICAL PRODUCT DEVELOPMENT

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#### ARTICLE INFO

##### Article history

Received 24/06/2024

Available online

31/07/2024

##### Keywords

Artificial Neural Networks,  
Recurrent Neural Networks,  
Drug repurposing,  
Clinical Trails,  
Polypharmacology,  
Physiologically Based  
Pharmacokinetic.

#### ABSTRACT

Artificial intelligence's usage in pharmaceutical technology has grown over time, and it may save time and money while offering a greater knowledge of the interactions between different formulations and process factors. Artificial intelligence is an area of computer science concerned with problem solving through the use of symbolic programming. Artificial intelligence (AI) employs personalized knowledge and learns from the solutions it generates to handle both particular and complex issues. Remarkable developments in processing power, along with advances in AI technology, have the potential to transform the drug development process. The pharmaceutical sector is now facing difficulty in continuing drug development programs due to higher R&D expenses and decreased efficiency. Artificial Neural Network (ANN) technologies are being developed for predicting relationships in data. Machine learning and deep learning are also being used to examine various machine parameters and regulate them accordingly to get the desired results. Thus, Artificial Intelligence programs serve as effective solutions for creating a medicinal product. They are also utilized in clinical studies to generate and evaluate data collected from patient information. As a result, in this article, we will discuss several applications of artificial intelligence in pharmaceutical product development, providing a clear picture of how AI has an efficient influence on the pharmaceutical industry.

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Please cite this article in press as **Imran A. W. Sheikh** et al. Artificial Intelligence: An Evolving Tool in Pharmaceutical Product Development. *Indo American Journal of Pharmaceutical Research*.2024;14(07).

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## INTRODUCTION

Artificial intelligence (AI) is a discipline of computer science that studies problem solving via symbolic programming. It has grown into a science of problem solving with numerous applications in business, health care, and engineering. The primary goal of this artificial intelligence is to identify practical information processing challenges and provide an abstract explanation of how to solve them. Such an account is referred regarded as a technique and correlates to a mathematical theorem. Artificial intelligence is a field concerned with the development and implementation of algorithms for data processing, learning, and interpretation<sup>[1]</sup>. Artificial intelligence encompasses several disciplines of statistical and machine learning, pattern recognition and grouping, and similarity-based approaches. AI is a thriving technology that has applications in many areas of life and industry. In recent years, the pharmaceutical industry has discovered unique and imaginative methods to leverage this sophisticated technology to assist tackle some of the most pressing challenges confronting the sector. In the pharmaceutical industry, artificial intelligence refers to the use of automated algorithms to do activities that would otherwise need human intellect. Over the last five years, the application of artificial intelligence in the pharmaceutical and biotechnology industries has transformed how scientists research new pharmaceuticals, treat diseases, and more.<sup>[1][2]</sup>

Artificial intelligence (AI) has caused a significant change in the pharmaceutical industry. It is widely used in all fields of healthcare. Many pharmaceutical firms are currently facing significant challenges in medication discovery and development due to a lack of research resources and excessive costs. As a result, AI technology is beneficial for efficient medication development.<sup>[3]</sup> This technology combines human intellect with computer processing. It is an advanced version of computer-aided approach that entails gathering information from many sources, developing rules to be followed for processing the essential information, and sketching potential outcomes to decide appropriate findings and conclusions. AI employs a variety of statistical approaches to make computer software and processes more like human behaviour. It is made up of components like machine learning and deep learning, which make it easier to deal with neural networks. Artificial intelligence approaches are used throughout the process, from identifying hit series to determining the lead molecule and eventually formulating the therapeutic molecule, including clinical trials. As a result, it is critical to increase innovation in the pharmaceutical business in order to produce drugs more accurately and quickly.<sup>[4][5]</sup>

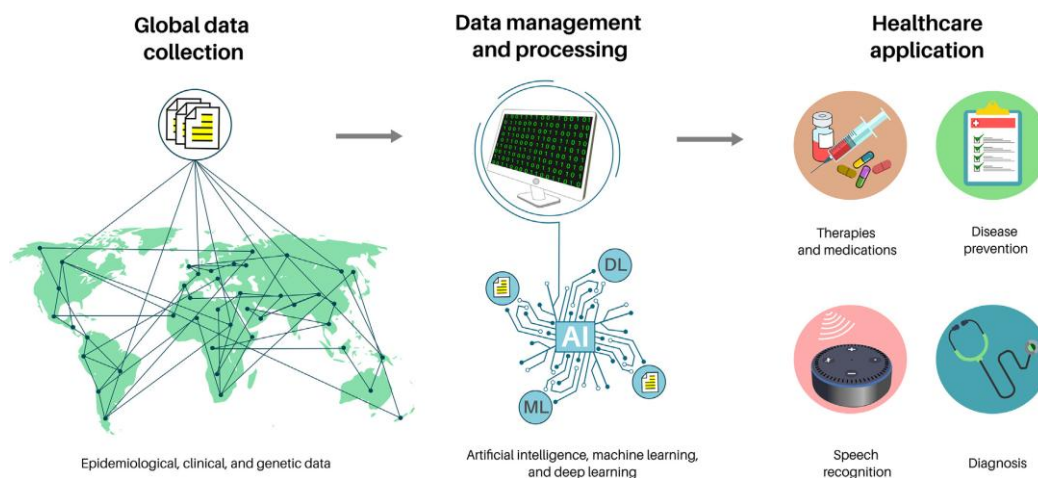
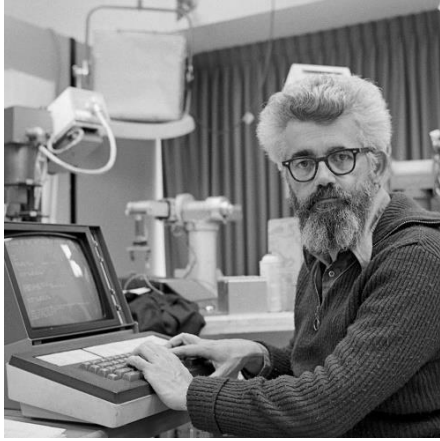


Fig No. 1: The application of artificial intelligence (AI) techniques in life sciences and healthcare. Data acquired from several patients may be combined and analysed with various AI technologies to enhance disease diagnosis, treatment, and prophylaxis. Voice and speech recognition can also be utilized by practitioners in clinical studies, as well as patients during consultations and clinical follow-up calls. AI may also aid with scientific hypothesis and article writing via dictation.<sup>[6]</sup>

## HISTORY OF ARTIFICIAL INTELLIGENCE

Alan Turing introduced the notion of using computers to emulate intelligent behavior and critical thinking in 1950. In the book "Computers and Intelligence," he developed a simple test (later known as the "Turing test") for determining whether computers can simulate human intellect. Six years later, John McCarthy defined artificial intelligence (AI) as "the science and engineering of making intelligent machines."<sup>[7]</sup>



**Fig No. 2: John McCarthy.**



**FigNo.3: Allen Newell and Herbert A. Simon.**

Allen Newell and Herbert A. Simon developed the computer software Logic Theorist in 1956, and Dartmouth College hosted the renowned conference. The income from the AI sector is expected to increase by up to tenfold between 2017 and 2022. The natural language processing industry, which includes applications such as text prediction and speech and voice recognition, is expected to increase by 28.5% in 2017. Worldwide income from big data and business analytics was \$122 billion in 2015, and it is predicted to exceed \$200 billion by 2020. Artificial intelligence has had a difficult past dating back to the 1950s. In 1997, IBM's Deep Blue computer defeated chess champion Garry Kasparov, leading to a shift in perception of the sport. In 2011, IBM's Watson supercomputer won the \$1 million prize on the US game show Jeopardy. Watson has now moved into healthcare and drug research, including a 2016 collaboration with Pfizer to speed immuno-oncology medication development. In December 2016, IBM and Pfizer released IBM Watson, a cloud-based tool that lets researchers uncover links across diverse data sets using dynamic visuals.<sup>[7][8]</sup>

## NETWORKS AND TOOLS IN ARTIFICIAL INTELLIGENCE

ANNs are complex structures created using the human nervous system paradigm. The basic components that comprise these networks, known as "perceptrons," are simplified representations of human biological neurons that simulate the transmission of electrical impulses in the human brain.<sup>[9][10]</sup>

ANN is made up of a network of nodes, each of which receives a separate input from a group of nodes before converting it to an output. Neural networks can be of several types, including single networks and multiple networks coupled together. There are several forms of artificial neural networks (ANNs), including multilayer perceptron (MLP) networks, recurrent neural networks (RNNs), and cellular neural networks.<sup>[9]</sup>

The MLP network offers a wide range of applications, including pattern recognition, optimization tools, process identification and control, and many more. These networks follow a specified design and are trained using supervised processes. Signals propagate in a single direction. These may be utilized as efficient methods for the generation of complex models, and hence serve as universal pattern classifiers.<sup>[9][11]</sup>

RNNs are regarded as a significant feature in the field of research and development. These are closed-loop networks whose outputs may be converted back into inputs. There are numerous varieties of RNNs, including Boltzmann and Hopfield. These closed-loop networks have various applications, including the capacity to memorize relationships and store information, foresee financial difficulties, estimate wind turbine output, and evaluate water quality.<sup>[9]</sup>

CNNs, or cellular nonlinear networks, are a collection of dynamic systems with local connections distinguished by their topology. They are commonly used in tasks like as image and video processing, biological system modelling, processing complicated brain operations, pattern recognition, and complex signal processing. All of these ANNs are simple, but they may also be more complicated, such as Kohonen networks, RBF networks, LVQ networks, counter-propagation networks, ADALINE networks, and many others.<sup>[9]</sup>

The selection and application of these ANNs to tackle a given difficult problem need thorough training and hands-on experience with standard operating procedures. These approaches can be either supervised or unsupervised learning techniques. The former learning approach involves feeding information about a correctly formed neural network and providing training on that basis, whereas the latter requires no prior knowledge of the answer. The supervised learning processes are classified into three types: iterative (repetitive changes to neuron parameters), probabilistic, and noniterative. Unsupervised learning processes may also be divided into competitive methods (selection of the strongest simulated neuron) and Hebb's rule methods (repeated simulation).<sup>[9]</sup>

AI technologies were also employed in the development of the Medicine and Engineering Designing Intelligence (MEDi) robot (developed at The University of Calgary in 2015 and produced by Aldebaran Robotics). The MEDi was created as a pain management tool that may provide support in more than 20 languages. The robot was created to explain the medical process to youngsters and teach them how to do it. Over time, it has expanded its uses beyond pain management to include rehabilitation, fundraising, and many more.<sup>[9][12]</sup>

Similar robots, known as TUG robots, were created by Aethon in 2004 to help hospitals transport drugs to patients, gather specimens, serve meals, haul loads, and clean rubbish. It features a well-designed network that calculates the optimum path to finish a certain activity, as well as extensive coverage to avoid obstructions.<sup>[9]</sup>

With the evolution of these technologies and networks, AI is gradually becoming an inseparable element of the healthcare system. These instruments can function considerably quicker than people and with fewer errors, potentially leading to rapid improvement in the healthcare sector.<sup>[9][12]</sup>

## DRUG DEVELOPMENT PROCESS



Fig No. 4: Stages of Drug Development.

## USE OF AI IN PHARMACEUTICAL PRODUCT DEVELOPMENT

The quest for successful new drugs is highly challenging, mainly due to the immense scope of chemical space, estimated to encompass around  $10^{60}$  molecules. However, the integration of AI technologies has significantly enhanced drug development by offering versatile tools applicable across various stages<sup>[13]</sup>. These include identifying and validating drug targets, designing new drugs, repurposing existing ones, enhancing R&D efficiency, analysing biomedical data, and optimizing patient recruitment for clinical trials. Leveraging AI presents a promising avenue to address the inefficiencies and uncertainties inherent in traditional drug development, all while reducing bias and human involvement in the process.

AI is also utilized in drug development for predicting viable synthetic pathways for drug-like compounds, as well as for forecasting pharmacological properties, protein attributes, efficacy, drug combinations, and associations between drugs and targets. Moreover, AI enables the identification of new pathways and targets through omics analysis, facilitating the discovery of novel biomarkers and therapeutic targets. Additionally, AI supports personalized medicine by leveraging omics markers and elucidates the relationships between drugs and diseases.<sup>[13][14]</sup>

Deep learning (DL) has showcased remarkable achievements in suggesting potent drug candidates and precisely forecasting their properties and potential toxicity hazards. Overcoming historical challenges in drug development such as analysing extensive datasets, streamlining compound screening to minimize standard error, and reducing the substantial R&D costs and time exceeding \$2.5 billion and over a decade are now feasible through AI approaches. With AI technology, new endeavours can be undertaken to aid in identifying novel drug targets, rational drug design, and repurposing existing drugs.<sup>[13][15]</sup>



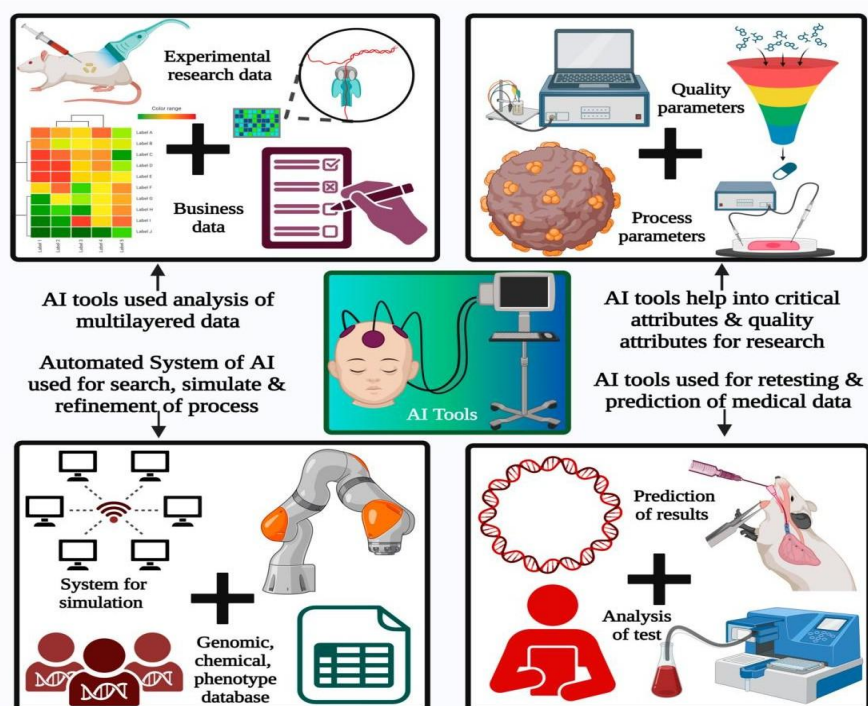


Fig No. 5: Application of AI techniques in the pharmaceutical industry. AI techniques are useful for analysing multilayered data. Automated AI systems are used to efficiently explore, simulate, and refine data and processes in research and product development. The system biology database, chemical database, genomic database, phenotypic database, and AI bots are used to explore drug models, forecast drug release and activity, and provide suggestions for viable drug delivery methods.<sup>[25]</sup>

#### AI in understanding the pathway or finding molecular targets

In drug development, AI has revolutionized the approaches for identifying pathways or targets to treat diseases. This transformation became feasible by integrating genomics data, biochemical characteristics, and target tractability<sup>[13][16]</sup>. For instance, a study investigated the feasibility of predicting therapeutic targets using a computational tool called 'Open Targets,' which utilizes gene-disease association data. The study reported that utilizing a neural network classifier, animal models displaying disease-relevant phenotypes achieved over 71% accuracy, providing significant predictive power. Additionally, IBM Watson for Drug Discovery, an AI platform, has uncovered five novel RNA-binding proteins (RBPs) associated with the pathogenesis of amyotrophic lateral sclerosis (ALS), a neurodegenerative disease.<sup>[13][17]</sup>

#### AI in finding the hit or lead

The integration of AI into the exploration of small drug-like molecules focuses on leveraging chemical space. Chemical space serves as a platform for identifying novel and high-quality molecules by computationally generating potential organic compounds. Furthermore, machine learning techniques and predictive model software aid in identifying target-specific virtual molecules and associating them with their respective targets, while optimizing safety and efficacy characteristics.<sup>[13]</sup>

AI systems play a crucial role in reducing attrition rates and R&D costs by minimizing the number of synthesized compounds subsequently tested in vitro or in vivo. Various in silico techniques, such as virtual ligand or structure-based design approaches, can be utilized alongside available data on small-molecule modulator probes or structural biology for profile selection. Deep learning proves beneficial when structural data are limited, allowing for the utilization of phenotypic data or algorithms based on disease biology or molecule networks.

Validated AI techniques hold the potential to enhance success rates in drug development, while those still under development require validation before integration into the drug development process. Synthesizing chosen molecules represents a critical phase in drug development, making AI invaluable for prioritizing molecules based on synthesis ease or developing effective tools for optimal synthetic routes.<sup>[13][18]</sup>

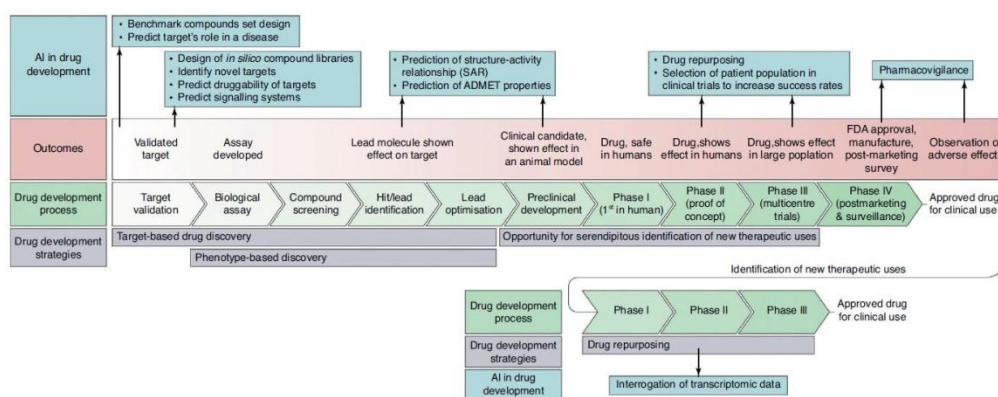


Fig No. 6: Use of artificial intelligence (AI) in the medication development process. The outcomes and tactics for each component of the drug development process are outlined. The use of AI at each step of drug development is also demonstrated.<sup>[20]</sup>

### AI in synthesis of drug-like compounds

Drug-like molecules are compounds that adhere to Lipinski's rule of five, which includes criteria such as molecular weight under 500 Da, limited hydrogen-bond donors and acceptors, and a calculated Log P value under 5. In synthesizing these molecules, chemists extensively employ retrosynthesis. This method involves recursively analysing target compounds to break them down into smaller, purchasable or readily preparable building blocks. The subsequent step is identifying reactions to transform these fragments into the target compounds. This phase is particularly challenging, as it is cumbersome for the human brain to sift through vast organic reaction databases to select the most suitable reactions. AI can significantly aid in predicting optimal reactions, addressing gaps that often lead to failures in organic synthesis, termed "out of scope" compounds. These gaps typically stem from unpredictable steric and electronic effects and an incomplete understanding of reaction mechanisms. While several computer-aided organic compound synthesis (CAOCS) systems exist to assist chemists in route selection, this aspect is not currently integrated into the computer-aided drug discovery (CADD) workflow.<sup>[13]</sup>

Seglaret.al. have introduced a novel AI platform called 3N-MCTS, which integrates three distinct deep neural networks with Monte Carlo Tree Search (MCTS) for computer-aided organic compound synthesis (CAOCS). This platform effectively sifts through potential building blocks, selecting only well-established reactions for synthesizing target compounds. Compared to traditional computer-assisted retrosynthesis systems, 3N-MCTS has demonstrated significantly improved speed and accuracy. It efficiently proposes viable synthesis routes devoid of unnecessary steps within a relatively short timeframe. However, there remains a gap in the quantitative prediction of enantiomeric or diastereomeric ratios and in devising plans for synthesizing natural products.<sup>[13][14]</sup>

### Predicting the mode-of-action of compounds using AI

The potential of having an AI platform capable of predicting both the on- and off-target effects as well as the *in vivo* safety profile of compounds before synthesis is a source of excitement for those involved in drug development, particularly medicinal chemists. Such platforms can significantly reduce drug development timelines, R&D costs, and attrition rates. Examples of these platforms include DeepTox, which predicts the toxicity of new compounds, and ProCTOR, which assesses the likelihood of toxicity in clinical trials. Enhancing the predictive accuracy of these platforms would require access to larger and more refined datasets on the toxicity and therapeutic profiles of diverse compound sets. However, achieving this necessitates a willingness to share data within the industry.<sup>[19]</sup>

Recently, an innovative AI tool called SPiDER was developed as an alternative to chemo proteomics to advance natural product drug discovery. As a proof-of-concept, SPiDER successfully predicted the molecular target of b-lapachone, a clinical-stage natural naphthoquinone with antitumor activity, identifying it as an allosteric and reversible modulator of 5-lipoxygenase (5-LO). This prediction was validated using a 5-LO functional assay. Another AI tool, Read-Across Structure-Activity Relationships (RASAR), which links molecular structures with toxic properties by mining a vast chemical database, was reported to accurately predict the toxicity of unknown compounds.<sup>[13][19]</sup>

### AI in selection of a population for clinical trials

An ideal AI tool for aiding clinical trials should be capable of identifying diseases in patients, pinpointing gene targets, and forecasting the effects of designed molecules, including both on- and off-target effects. One innovative AI platform, AiCure, has been developed as a mobile application to monitor medication adherence in a Phase II trial involving individuals with schizophrenia. Results indicated that AiCure improved adherence by 25% compared to traditional methods like modified directly observed therapy.<sup>[20]</sup>

The process of patient selection for clinical trials is crucial. By examining the correlation between human-relevant biomarkers and *in vitro* phenotypes, a more predictable and quantifiable assessment of therapeutic responses in specific patients can be achieved. The advancement of AI approaches to identify and predict human-relevant biomarkers of diseases enables the recruitment of precise patient populations for Phase II and III clinical trials. Incorporating AI predictive modelling in patient population selection could enhance the success rate of clinical trials.<sup>[20][21]</sup>

### AI in drug repurposing

AI enhances the drug repurposing process, making it more appealing and practical. Repurposing existing drugs for new diseases offers the advantage of allowing the new drug to skip Phase I clinical trials and toxicology testing and proceed directly to Phase II trials for a different indication. Recent reports have highlighted *in silico* methods that predict the pharmacological properties of drugs and identify potential repurposing opportunities using transcriptomic data across various biological systems and conditions through DL applications. These methods rely on high-level data representations utilizing deep neural networks (DNNs), which are sophisticated multilayer systems consisting of interconnected artificial neurons capable of various data transformations. Aliper *et al.* demonstrated that DNNs could effectively classify complex drug action mechanisms at the pathway level, thereby categorizing drugs based on their functional class, efficacy, therapeutic use, and toxicity<sup>[13][22]</sup>. Moreover, advancements in precision medicine have led to the development of next-generation AI capable of designing drug molecules using generative adversarial networks (GANs). GANs, a remarkable technology, leverage DL to generate realistic images from text descriptions, enabling tasks beyond data analysis, such as imagining or creating new data modeled on real data. Fundamentally, the GAN technique involves an adversarial game between two DNNs, where one evaluates the output of the other iteratively, allowing the two networks to learn and improve their ability to generate more accurate molecules.<sup>[13]</sup>

Another advanced AI method utilized in computational medicine is reinforcement learning. This AI technique offers the advantage of being less reliant on learning from extensive datasets, allowing networks to recognize effective strategies in drug molecule design. Zhavoronkov's research team has developed algorithms capable of filling in missing features from incomplete datasets and deciphering differences between normal and diseased profiles within complex data. A notable area of focus is the potential of AI in creating drugs with reduced side effects. Moreover, the AI algorithm is undergoing training to distinguish between cardiotoxic and non-cardiotoxic drugs using gene expression data obtained from cells exposed to various drugs. Currently, the team is pitting their AI-designed molecules against those crafted by chemists. An effort has been made to capture the intrinsic knowledge that aids seasoned medicinal chemists in identifying promising drug candidates, employing mobile electroencephalography to measure responses to a molecule's structure and numerical properties<sup>[13][23]</sup>. Additionally, the research aims to uncover any biases in the types of drug molecules favored by chemists, which may not be evident in AI-designed molecule selection.

### AI in Polypharmacology

The prevailing approach in drug development has shifted from the 'one-disease–one-target' model to the 'one-disease–multiple-targets' paradigm, known as polypharmacology, due to a more profound comprehension of disease processes at the molecular level. Various databases like ZINC, PubChem, Ligand Expo, KEGG, ChEMBL, DrugBank, STITCH, BindingDB, Supertarget, and PDB offer a wealth of information on molecular pathways, crystal structures, binding affinities, drug targets, disease relevance, chemical properties, and biological activities. AI can be leveraged to explore these databases to design polypharmacological agents effectively. A recent success story in this domain involves the development of Deep DDI, a computational platform aimed at enhancing understanding of drug-drug interactions, their mechanisms, and predicting alternative drugs for clinical use without adverse health effects.<sup>[13][24]</sup>

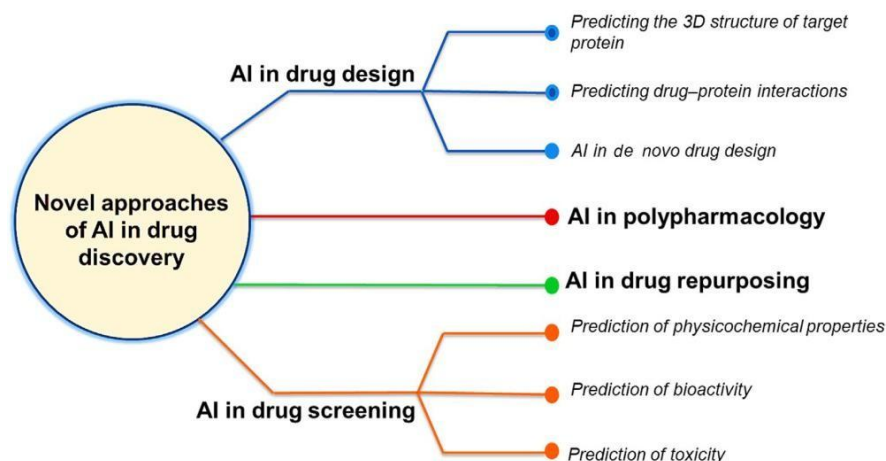


Fig. No. 7: Applications of AI In Drug Development<sup>[9]</sup>.

### CHALLENGES TO ADOPTION OF AI IN PHARAMA

While AI has the potential to significantly transform the pharmaceutical sector, adoption is not without challenges.



### Challenges that pharmaceutical businesses confront when attempting to implement AI:

1. Technology unfamiliarity - Because of its novelty and esoteric nature, AI remains a "black box" for many pharmaceutical organizations.
2. Inadequate IT infrastructure - Current apps and infrastructure were not created with AI in mind. Even worse, pharmaceutical companies must invest a lot of money to improve their IT systems.
3. Pharma businesses must work hard to compile and evaluate free text data. Despite these limits, one thing is certain: artificial intelligence is already altering biotechnology and pharmaceuticals. Maybe five years from now, Pharma will see artificial intelligence as a fundamental, everyday technology. <sup>[1]</sup>

### Artificial Intelligence in Pharmaceuticals is a good idea:

The pharmaceutical industry may speed innovation by using technology breakthroughs. The most recent technical innovation that comes to mind is artificial intelligence, which is the creation of computer systems capable of doing activities that would typically need human intellect, such as visual perception, speech recognition, decision-making, and language translation. According to an IBM estimate, the whole Healthcare domain had over 161 billion GB of data in 2011. With so much data accessible in this arena, artificial intelligence may be of great use in evaluating it and delivering results that will aid in decision making, saving human effort, time, and money, and thereby saving lives. Machine learning and artificial intelligence may accurately forecast epidemic outbreaks by studying their history, analysing social media activity, and predicting their location and timing. <sup>[1]</sup>

Aside from the aforementioned use-cases, there are countless others, including:

1. Personalizing therapy.
2. Contribute to the development of innovative tools for patients, clinicians, and other stakeholders.
3. Clinical trials research: Using predictive analytics to find trial participants via social media and clinic visits.

### FUTURISTIC OVERVIEW

In the future, AI stands poised to transform the pharmaceutical industry by expediting drug discovery and development processes. Advanced virtual screening techniques will swiftly sift through vast chemical libraries to identify potential therapeutic candidates with specific attributes, hastening the identification of lead compounds. AI-driven personalized medicine could analyse genomic, proteomic, and clinical data to categorize patients, forecast treatment responses, and tailor medications accordingly. Scientists may utilize deep learning and generative models to design novel compounds with precise target-binding properties, thereby enhancing drug efficacy while minimizing adverse reactions. Moreover, AI will enable the formulation of patient-specific doses by optimizing medication compositions and delivery methods based on individual parameters such as age, weight, genetics, and health status. Furthermore, AI algorithms will revolutionize safety assessments by forecasting potential side effects and toxicity of drug candidates. <sup>[25]</sup>

AI-driven monitoring systems will enable remote patient care and enhance medication adherence by utilizing wearable devices and sensors to collect continuous data. This data will be processed by AI algorithms to suggest personalized therapies and improve patient compliance. Additionally, AI will enhance the design of clinical trials, patient selection, and recruitment processes. By leveraging electronic health records, biomarkers, and genetic profiles, AI algorithms will identify suitable patients, reduce trial expenses, and expedite approval timelines.

AI models will play a crucial role in real-time monitoring and controlling key parameters to enhance continuous manufacturing processes. Through data analysis and feedback mechanisms, AI algorithms will streamline pharmaceutical manufacturing, ensuring uniformity and efficiency. Furthermore, AI will leverage vast amounts of data to inform regulatory decisions, aiding regulatory bodies in expediting medication approval processes and enhancing safety standards. <sup>[25][26]</sup>

The utilization of artificial intelligence across various healthcare domains is experiencing continuous growth, encompassing functions ranging from triage and clinical risk prediction to diagnosis. AI applications in clinical settings hold promise for enhancing diagnostic accuracy and healthcare efficiency. Given the substantial resources invested in medication research and development, there is a pressing need for innovative methodologies and strategies. Artificial intelligence presents significant opportunities in medicine, including the analysis of extensive multivariate data, addressing complexities in creating effective medication delivery systems, improving decision-making accuracy, disease classification, and modelling.



It also aids in establishing correlations between formulations and processing parameters, optimizing dosage ratios, expediting drug development, predicting drug bioactivities and interactions, understanding cellular responses, evaluating the efficacy of combination therapies, treatment outcomes, and more. While AI and machine learning hold significant potential in revolutionizing medication delivery to enhance the effectiveness of infectious disease treatment, their practical applications in this area remain limited, particularly within therapeutic settings. Various AI methods employed in drug delivery for treating infectious diseases, including Boost, k-nearest neighbours, decision trees, random forest, Naïve Bayes, artificial neural networks (ANN), Feedback System Control (FSC), support vector machines (SVM), Set Covering Machine (SCM), and logistic regression, have not undergone extensive evaluation or adoption in clinical settings. This indicates significant obstacles in translating AI into clinical practice for medication administration in the treatment of infectious diseases.

The integration of machine learning and artificial intelligence with PBPK (Physiologically Based Pharmacokinetic) modelling serves as crucial tools in drug development and the assessment of environmental chemical risks<sup>[27]</sup>. A recently developed PBPK model has been utilized to elucidate the processes involved in the entry of chemicals into the body, drug bioavailability, inter-tissue drug movement, and drug metabolism and elimination through mathematical representation. When assessing the toxicity of various classes of nanomaterials, PBPK-based toxicity models are deemed most appropriate. However, due to the lack of well-defined chemical ADME (Absorption, Distribution, Metabolism, and Excretion) routes and mathematical formulations, creating mechanistically valid PBPK models for novel compounds with limited prior knowledge poses significant challenges and complexities. The emergence of Neural-ODE algorithms represents a significant stride in constructing PBPK simulations for new medications. These algorithms enable the learning of governing ODE equations directly from pharmacokinetic (PK) data, bypassing the need for extensive prior knowledge. This advancement, alongside AI methodologies like deep neural networks, holds promise in addressing current challenges in PK and PBPK modelling. These technologies can enhance drug discovery, development, and human health risk assessment for environmental chemicals. However, realizing the full potential of AI in PKPD hinges on a thorough grasp of underlying scientific principles. Achieving this demands the establishment of robust regulations to curb misuse while fostering growth. Such an endeavour necessitates collaboration among pharmaceutical firms, regulatory bodies, and healthcare professionals, including doctors, nurses, pharmacists, and data scientists.<sup>[25][26]</sup>

Although the prospects outlined in this futuristic perspective are compelling, it's crucial to acknowledge the hurdles concerning data reliability, regulatory structures, and ethical standards that must be overcome for AI to fully benefit pharmaceutical product development. Nevertheless, with ongoing progress and partnerships among industry, academia, and regulatory entities, AI-driven advancements hold the promise of transforming the pharmaceutical sector and enhancing patient outcomes in the foreseeable future.<sup>[26][27]</sup>

## CONCLUSION

Human beings are the most advanced machines that have ever been made. The human brain is striving hard to build something that is far more efficient than a human person in doing any given activity, and it has been quite successful in doing so. AI solutions like as Watson for Oncology, pull robots, and robotic pharmacies have significantly changed the field. As the healthcare sector grows, it will require increasingly complex and technologically advanced infrastructure. Artificial intelligence is the development and implementation of algorithms for data analysis and interpretation.

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