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# Artificial Intelligence in Drug Discovery & Development

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## ABSTRACT

Drug discovery and development is a complex, costly, and time-intensive process involving target identification, optimization, preclinical evaluation, clinical trials, regulatory approval, and post-market monitoring. Advances in artificial intelligence (AI) are transforming this landscape by enabling data-driven decision-making, reducing timelines, and improving predictive accuracy across the pharmaceutical pipeline. AI supports target identification through genomic and proteomic data analysis, enables de novo drug design with generative models, and aids property prediction and toxicity study using machine learning. In preclinical Trails, AI improves pharmacokinetic and pharmacodynamic modeling, predicts ADMET parameters, and supports the 3Rs principle by reducing animal use. Clinical research benefits from AI-driven patient recruitment, adaptive trial design, adherence tracking, and decentralized execution. Manufacturing and formulation are optimized with AI-based modeling, automation, and quality control. Regulatory review increasingly integrates AI for dossier evaluation, real-world evidence analysis, and safety monitoring, while post-marketing surveillance applies NLP and machine learning to detect adverse drug reactions and safety signals from diverse data sources. Despite challenges in data quality, interpretability, ethics, and regulatory acceptance, AI promises to reduce costs, improve efficiency, accelerate innovation in drug discovery and development. Future progress requires explainable, transparent, & globally harmonized AI solutions.

**Keywords**: Artificial intelligence, Drug discovery, Machine learning, Pharmacovigilance, ADMET prediction, Clinical trials

## INTRODUCTION

drug discovery is a procedure aim to study a small synthetic compound or a large biological molecule for extensive assessment as a prospective therapeutic agent. Generally, modern pharmaceutical research encompasses identifying the illness to be addressed and its unfulfilled medical requirement, selecting a molecular target amenable to intervention and confirming its relevance, developing laboratory assays, then using high-throughput screening to assess compound libraries against the target to find active candidates, followed by optimization of these hits to produce lead substances that show sufficient strength and selectivity for the specific biological target in laboratory tests and which demonstrate effectiveness in disease models using animals. Afterwards, the lead molecules undergo further refinement to enhance their effectiveness and pharmacokinetic profiles prior to progressing to medicine development. The drug development process can be divided into preclinical and clinical phases. In preclinical development, toxicology and safety pharmacology investigations of the candidate are performed to define the highest safe concentrations in animal subjects and assess the risk of harmful effects of the investigational medication. Additionally, manufacturing economics and optimal formulation strategies are determined for the candidate medicine Should the candidate display adequate effectiveness and safety in preclinical studies, approval is sought from regulatory authorities to begin clinical evaluations, wherein the safety and efficacy of the medicine candidate are assessed in preliminary and confirmatory trials. Bringing original therapeutics to fruition is both time-consuming and costly, of to introduce a new medication to market. Over time, the number of novel medicines receiving marketing authorization has declined due to increased regulatory scrutiny regarding safety and efficacy, which inflates costs and lengthens timelines. In addition, leadership within the pharmaceutical sector seeks to curb the hazards linked to medicinal exploration and product development. National healthcare systems are under economic strain from pharmaceutical-related expenses, adversely affecting the pricing of drugs. Patent expirations and subsequent substitution by generics have reduced profitability and hindered the growth of the drug industry, lowering

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investment in innovative research Another emerging concern is the negative environmental footprint of pharmaceuticals, prompting regulatory directives to mitigate these effects.


**Role of AI in drug discovery and development:**

Artificial intelligence plays a transformative role throughout drug discovery and development process by significantly improving efficiency, accuracy, and speed.

**Key contributions of AI include**:

- Target identification and validation
- Preclinical development and toxicity prediction
- Clinical trial optimization
- Role of Al in Regulatory Review
- Post market monitoring

**Target identification and validation:**

Artificial intelligence examines vast biological and biomedical datasets to pinpoint potential drug targets, such as proteins or genes linked to various diseases. Platforms like DeepMind's AlphaFold forecast three-dimensional protein structures, transforming target comprehension and drug discovery. The capability of AI to anticipate drug–target interactions has also been employed to facilitate the repositioning of existing drugs and minimizing polypharmacology. Repositioning a pre-approved drug directly qualifies it for Phase II clinical investigations. This strategy also lowers costs, as reintroducing an already available drug requires about for launching a new chemical entity. The Guilt by association method can be applied to predict novel relationships between drugs and diseases, relying either on knowledge-driven or computationally generated networks. In computationally designed networks, machine learning methods are extensively applied, including techniques such logistic regression. Logistic regression platforms like predict, space, and other ML models consider drug–drug and disease–disease similarities, molecular target resemblance, chemical structures, and gene expression data while repurposing drugs.[1]

Cellular network–based deep learning frameworks have been investigated to identify therapeutic applications of topotecan, currently used as a topoisomerase inhibitor. It may also be repurposed for multiple sclerosis therapy by inhibiting the human retinoic acid receptor–related orphan receptor-gamma. This platform is under a provisional US patent. Self-organizing maps, which fall under unsupervised ML approaches, are also applied in

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drug repurposing. They adopt a ligand-based strategy to identify novel off-targets for drug libraries by training the model on known compounds with validated biological functions, later analysing different candidates.

In a recent study, deep neural networks were utilized to repurpose existing drugs with established activity against, HIV, and influenza virus, as well as compounds known as 3C-like protease inhibitors. In this work, extended connectivity fingerprints, functional-class fingerprints, and the octanol–water partition coefficient were incorporated to train the AI system.

**Generation of novel compounds**: AI designs innovative drug candidates with favorable characteristics by learning from existing molecular data. This expedites the development of molecules optimized for solubility, efficacy, and other features, moving beyond conventional trial-and-error methods.

**Molecular simulations and property prediction:** AI facilitates in silico modeling of drug–target interactions and provides precise predictions of pharmacological properties (toxicity, bioactivity, ADMET profile), minimizing reliance on expensive and time-intensive laboratory experiments.

**Drug candidate prioritization and synthesis pathway design:** AI ranks lead molecules for subsequent evaluation and proposes efficient synthetic routes, thereby streamlining the overall drug development pipeline. [2]

**AI for large-scale data analysis and network-based target identification:**

Ai models particularly like [ML learning and DL [beep learning, algorithms. Get process genomic proteomic and transcriptomic data to know the key biomarkers and a receptors target. It types like enquires Receptors, Ion channels, transporters, ε protein-protein interactions. the data-sets are too lengthy and complex. For the traditional analytical methods to maintain effectively by taking advantage of AI researchers can defined different types of biological data, identify related patterns. And prioritize main targets based on their biological significance and draggability excels in network. & identifying targets that are critical to disease progression. Deep Learning [DL] Model's as convolutional networks CNNS [3]

Recurrent neural networks (RNN'S) con be trained to study drug target; interactions used to gain knowledge of new ones (or) drug [GANS Generative adversarial network used to show the design new molecules. That are enhanced to bind to specific network nodes and offering AI driven approach to new drug design. In RL] Reinforcement learning models used at finding novel molecules with distributions different from the training data sets, maxing it happened to know unknown chemical spaces and optimize for specific properties These models are particularly attractive in new system pharmacology approaches [4].

**High-throughput screening and data analysis:**

The one of the main advantages of AI in target identification is its capacity to analyze bulk and complex datasets, these data evolution reflects the traditional methods. Ai driven reach not only streamline the target drug discovery method and give insights into the complex biological network which are plays major Role components of the oncogenic processes. [5]

**Preclinical development and toxicity prediction:**

In the process of preclinical development the AI plays an important role in predictive modeling by stimulating biological responses to drug candidates It evaluates toxicity risks, unintended. Effects & overall safety using in computation all experiments before any laboratory (or) animal testing. This validation help eliminate weak & unwanted compounds to save significant cant time cost and ethical concerns collaborate with traditional preclinical trails. And also Al models can help to predict & find pharmacokinetics &. Dynamics (PD) emulating how drugs will interact with the human body, like absorption, distribution, Metabolism & excretion patterns. Over and above that AI provides to the" 3 RS" [replace, reduce, reline] of the animal use in the research by increasing the efficiency and accuracy of safety modeling, thereby reducing the Assurance on extensive. [6]

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In these preclinical trials they are two types of methods;

1.In vitro method

2.In vivo method

**1.In vitro method:**

As a popular method in drug discovery, cell-free systems show various advantages such as fast processing, microscale operation, high throughput, and reproducible as well as stable screening results. However, molecular test models are generally built for particular targets and thus only provide limited information on target interactions. In addition, the pharmacological activity of some compounds in a living organism is extremely intricate, with multi-layered interactions that cannot be reasonably predicted by using biochemical assays. Therefore, single-molecule, high-throughput drug screening technologies are no longer adequate to meet the new demands on drug discovery. To surpass this limitation, more biologically relevant cell-based screening assays have emerged and are now largely used to forecast organism-level responses to drugs. Additionally, cell culture systems are frequently selected as models to evaluate cellular toxicity and have been proven to be of paramount importance in drug development.[7]

**In vivo method:**

In vivo methods in preclinical research refer to experimental studies conducted on living animals to evaluate the pharmacological and toxicological properties of new drug candidates before they are tested in humans. These studies are essential because they provide crucial information on how a drug behaves in the complex biological system of the whole body, which cannot be completely understood through in vitro (cell-based) or in silico (computer-based) models. In vivo experiments help determine pharmacokinetic parameters such as absorption, distribution, metabolism, and excretion (ADME), as well as pharmacodynamics responses that show how the drug interacts with its biological targets to produce therapeutic effects. They are also used to assess drug efficacy using various disease models. Moreover, toxicological studies are an integral part of in vivo testing and include acute, sub-acute, chronic, reproductive, genotoxicity, and carcinogenicity evaluations to identify safe dose ranges, organ-specific toxicity, and long-term safety concerns. Safety pharmacology studies further examine the effects of a drug on vital systems such as cardiovascular, respiratory, and central nervous system functions. These studies are strictly regulated by ethical guidelines and must comply with Good Laboratory Practices (GLP) and animal welfare regulaton . Although in vivo studies are expensive, time-consuming, and sometimes limited by differences between animal and human physiology, they remain indispensable in drug development because they provide the most reliable predictions of a drug's efficacy and safety in humans and form the foundation for submitting an Investigational New Drug (IND) application .[8]

**Pharmacokinetic Parameters (Absorption, Distribution, Biotransformation and Excretion)**

Drug absorption refers to the process through which drugs enter the circulation from the site of administration. Bioavailability is an important pharmacokinetic feature that encapsulates the amount of absorption. Predicting the bioavailability of a molecule may enable the medicinal chemist to optimize its absorption properties. One group of researchers collected a dataset of compounds and used the MLR paradigm to predict bioavailability supported by structural fingerprints along with molecular descriptors Genetic function approximation method was used to select the set of molecular descriptors used for process training in an automatic fashion, and the results achieved a strong predictive success respectively.[9]

Distribution of drugs is the process through which drug molecules migrate in blood to interstitial fluid and intracellular fluid as a result of drug penetration . The steady-state distribution of a drug is the ratio of its dose in vivo to its steady-state plasma concentration . The represents the extent to which an active molecular medicine is spread out in the tissue and is actually a very important parameter to evaluate drug distribution. Predicting volume of distribution (VDss) can help medicinal chemists to introduce structural modifications for better pharmacokinetic profiles. One study team collected a dataset of molecules and constructed Partial Least Squares (PLS) and Random Forest (RF) models to predict VDss. The presage results of their algorithm on the external test set were disappointing, with only roughly 50% of the molecules being within two-fold error. Apparently, it

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is not possible to presage VDss value solely from molecular architectural information because there just so happen to be several unidentified parameters which can affect VDss.[10]

After the drug is administered into the body, it will first face the metabolic process with attendant loss of drug effects, or, in some cases, formation of toxic metabolites. Prediction of the site of biotransformation with maximum accuracy can help in the structural optimization for ensuring the metabolic stability of the moiety. An enormous amount of information relating to drug metabolism has been harvested, and various ML schemes have been used to predict the locations where molecules are bio-transformed by different metabolic enzymes based on a neural network strategy, can provide the prediction of the location of small molecules biotransformed with a coarseness of 87% accuracy . Further, the "XenoSite"scheme also utilizes a neural network trained on an enormous database of biotransformation

Drug excretion is how drugs and their bio-transformed metabolites are eliminated from the system. Bio-transformed metabolites of drugs are usually water-soluble and can easily be eliminated from the body whereas some drugs can be eliminated directly without biotransformation. Utilized the Principal Components Analysis (PCA) method to predict primary clearance pathway and the algorithm had good discrimination results among different methods and a predictive accuracy of 84% . Based on the elimination process prediction paradigm, the group utilized the algorithm to predict the gross human clearance and the paradigm performed well and was similar to animal scaling methods.[11]

**Toxicity and the ADME/T Multi-Task Neural Network**

During drug development, pre-clinical and clinical toxicity contributes to the elimination of about 33% of top moieties. Therefore, predicting the toxicity of compounds is priceless in aiding the optimization of lead moieties and cutting the risk of loss during the process of drug development. Traditionally, drug toxicity properties (e.g., hepatotoxicity and nephrotoxicity) are predicted by axiom-based expert knowledge and design warnings, which seem to create false positives and are unable to capture broadly all the required structural features. Now, due to the ability of processing diverse chemical entities and the merit of extracting feature dimensions automatically, the DL algorithms produce strong performance on toxicity prediction. As an example, according to the "Molecular Graph Encoding-Convolutional Neural Networks. Designed a sharp oral toxicity forecast paradigm, and the forecasting results were better than the previously reported method. In the MGE–CNN framework, the molecular enciphering, feature extrication and model construction is performed by techniques similar to the training of neural networks. Also, the MGE–CNN algorithmic framework is rather flexible because molecular fingerprints can be customized according to the particular problems.[12] A research team mapped toxicological fingerprints' properties back to atomic levels and collected some highlighted pieces that adhere to structural flags described in the "ToxAlerts" . Accordingly, by analogy with Duvenaud's model is also understandable. The other group developed a multi-task DNN algorithm called "DeepTox" to predict the toxic effects and the "DeepTox" system outright dominated many others in the Tox21 challenge . Accepting the same criteria, the multi-task neural network algorithm was trained to predict many different independent discrete tasks that are remarkably related. As compared to single-task neural network, the performance of multi-task neural network is typically better due to sharing of the requirements of different assignments in supporting the multi-task algorithm for imprinting more known characteristics.

Pharmacokinetic processes (drug absorption, distribution, biotransformation, excretion) and drug toxicity in the human system bear some resemblance to each other and the multitasking neural networks can improve the predictive ability of such tasks. Vertex Pharmaceuticals' ADME/T experimental datasets have been used to compare the performance of single-task and multi-task neural networks, and their results suggested that multi-task algorithms would perform better as expected.[13]

**Clinical trial optimization**:

AI supports the design and conduct of clinical trials by predicting compound efficacy and safety, improving success rates while reducing costs.AI-driven drug discovery has already led to milestones such as the first AI-designed drug entering clinical trials, AI-discovered molecules progressing rapidly through development, and FDA recognition for AI-generated drugs. Studies show AI-identified drug candidates often have a higher success

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rate in trials compared to traditional methods. Regulatory bodies like the FDA's Center for Drug Evaluation and Research (CDER) are actively developing frameworks to responsibly integrate AI into drug development, ensuring safety and efficacy alongside fostering innovation.

Overall, AI's role spans from early discovery—decoding biology and generating molecules—to late-stage development and regulatory science, substantially reducing time, costs, and attrition rates in bringing new drugs to market. [14]

**Innovating clinical Trails:**

Clinical trials are designed to prove the efficacy and safety of a drug in humans for a particular disease and require 6–7 years along with a huge cost outlay. But only 10% molecules evaluated in such trials get full approval, which is a huge failure to the industry .Such losses could result from inappropriate patient selection, lack of technical infrastructure, and inadequate facilities. But, with the gigantic amount of digital medical data available, these drawbacks can be limited by using AI.[15]

Patient recruitment takes up approximately 33% of the clinical trial period. The success of a clinical trial could be made easier by proper patient enrollment. which on the cContrary accounts for ~86% of non-success situations . AI could assist in selecting a diseased population for Phase II and III clinical triaL participation using patient-pertinent genome-exome sequencing could enable sophisticated analysis of the current drug targets available in the selected subjects. Preclinical examination of molecules ae identification of lead compounds before clinical trials are initiated using adjunct capabilities of AI, such as predictive ML and other differencing algorithms, assists in the advanced prediction of lead molecules that would pass the cut in clinical trials in the target patient population . [16] Patient dropout in clinical trials is responsible for the non-fruition of approximately one-third of clinical trials and causes additional enrolment requirements for the conclusion of the trial, resulting in inefficiency and wasted resources. These problems can be avoided by strict monitoring of the patients and making them adhere to the protocol of the clinical trial. Mobile applications have been made available by "AiCure" that monitored normal use of medication in schizophrenia patients during a Phase II clinical trial, which resulted in subsequent increase in the compliance rate of patients by 25%, ensuring a successful end of the clinical. [17]

AI is greatly transforming clinical trails strengthening efficiency and success percentage it upgrade patient recruitment and ordering by evaluating electronic health records and other data to quickly assess patient eligibility, identify suitable trail, participants. & Startify patient based on genetic profiles (or) disease progression. At also streamline trail design by studying historical data to recommend ideas procedures, endpoints and timelines, where Ai simulates trail designs and Outlook based on historical data, & reducing trails Failures[18].

The AI helps to increase efficiency &. support decentralized. Clinical trio [DCT's] the use of the synthetic control arms [SCAS), where Al and data analytics standard, Real world data [RWD] and historical trial data to simulate control groups like cost challenges collabrate with traditional trails And the method of digital twins where Ai creates virtual replies of patients of disease models for virtual treatment testing further enhance strategies and reduces risks. And the Idea of using of analytical models to partially (or) totally replace human (or) animals testing, as suggested by the development of digital twins & synthetic control arms represents a significant shift while offering immense ethical benefits, such as reduced. animal testing & reference groups and pro advantages in terms of speed. & cost, this development raises deep questions about the regulatory acceptance & validation of purely. in silico evidence[19]

**AI in the development of pharmaceutical products:**

Identification of a new drug molecule demands its incorporation later in an appropriate dosage form with desirable delivery properties. Here, AI can substitute the traditional trial and error method. Different computational tools can solve issues faced in the formulation design field, like stability, dissolution, porosity, Decision-support tools utilize rule-based systems to choose the type, nature, and amount of the excipients according to the physicochemical properties of the drug and work on a feedback mechanism to monitor the

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whole process and intermittently adjust it .[20] The combined Expert Systems (ES) and ANN to design a hybrid system for development of direct-filling hard gelatin capsules of piroxicam according to its dissolution profile specification The modern expert system (MES) decides and makes recommendations for formulation development depending on the input parameters. On the other hand, ANN applies backpropagation learning in order to connect formulation parameters with the expected response, controlled together by the control module, to make formulation development trouble-free.Different mathematical tools, for instance, computational fluid dynamics (CFD), discrete element modeling (DEM), and the Finite Element Method have been employed to investigate the effect of the flow characteristic of the powder on the die-filling and tablet process compression The effect of tablet geometry solution profile can also be analyzed using CFD . The integration of these mathematical models with AI may turn out to be of huge assistance in the quick production of pharma products.[21]

**AI in pharmacy product manufacturing:**

With growing complexities in manufacturing processes along with growing need for efficiency and improved product quality, new manufacturing systems are attempting to impart human knowledge to machines, changing the manufacturing practice constantly. The use of AI in manufacturing can serve as an impetus for the pharmaceutical sector. CFD is an example, as it employs Reynolds-Averaged NavierStokes solvers technology that investigates the effect of agitation and stress levels within various equipment taking advantage of the automation of most pharmaceutical processes. Comparable systems, like direct numerical simulations and large simulations, encompass sophisticated methods to solve complex flow issues in production . [22] The new Chemputer platform assists digital automation for synthesis and production of molecules, using various chemical codes and functioning through the usage of a scripting language referred to as Chemical Assembly . It was implemented successfully for the synthesis and production of sildenafil, diphenhydramine hydro-chloride, and rufinamide, with yield and purity quite comparable to manual synthesis . The approximate completion of granulation in granulators having capacities from 25 to 600 l can be accomplished effectively by AI technologies . The technology and neuro-fuzzy logic mapped critical variables to their responses. They obtained a polynomial equation for the prediction of the amount of the granulation fluid to be added, needed speed, and the impeller diameter of the both geometrically similar and dissimilar granulators digital evaluation model DEM has extensively been applied in the pharmaceutical sector, the influence of changing blade speed and form, forecasting the potential path of the tablets in coating process, together with analysis of the time spent by tablets under the spray zone ANNs, along with fuzzy models, investigated the relationship between machine parameters and the issue of capping to minimize tablet capping on the production line.Meta-classifier and tablet-classifier are computer programs that assist in controlling the quality level of the final product, reflecting a potential mistake in the production of the tablet . A patent application has been made, showing a system with the ability to find the most dainty mix of drug and dosage regimen for each patient, with a processor that receives the information of the patient, and designs the transdermal patch accordingly [23]

**AI in quality control and quality assurance:**

Manufacturing of the desired product from the raw materials includes a balance of various parameters . Quality control tests on the products, as well as maintenance of batch-to-batch consistency, require manual interference. This might not be the best approach in each case, showcasing the need for AI implementation at this stage . The FDA amended the Current Good Manufacturing Practices (cGMP) by introducing a ‘Quality by Design’ approach to understand the critical operation and specific criteria that govern the final quality of the pharmaceutical product used a combination of human efforts and AI, wherein preliminary data from production batches were analysed and decision trees developed. These were further translated into rules and analyzed by the operators to guide the production cycle in the future studied the dissolution profile, an Indicator of batch-to-batch consistency of theophylline pellets With the aid of ANN, which correctly predicted the dissolution Of the tested formulation with an error of <8% . [24]AI can also be implemented for the regulation of in-line Manufacturing processes to achieve the desired standard of the Product . ANN-based monitoring of the freeze-drying process Is used, which applies a combination of self-adaptive evolution Along with local search and backpropagation algorithms. This can Based To predict the temperature and desiccated-cake thickness at a Future time point for a particular set of operating conditions, Eventually helping to keep a check on the final product quality .An automated data entry platform, such as an Electronic Lab Notebook, along with sophisticated,

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intelligent techniques, can Ensure the quality assurance of the product . Also, data mining And various knowledge discovery techniques in the Total Quality Management expert system can be used as valuable approaches in Making complex decisions, creating new technologies for intelligent quality control.[25]

**Toxicology prediction:**

The AI tool helps to study and collecting data on toxicology, and to boosts, the efficiency and Accuracy. In. Addition Statistical modeling was detailed discussed as a method di to give more detailed. risk characterizations than traditional. It is safe or unsafe And these AI modals tools have been – developed for predation of toxicological on outcomes and drug safety. [26] Using like [DL] deep learning, Al models can helps to predict and study the effects of chemicals (or) drugs are more Exactly. And the benefit of reducing reliance on animal use. Extensibility is a benefit of At in regulatory workflows. And many of the regulations follow an Exacting & short timeline. Al can process a large volume of data quickly to study priority chemicals for further testing or to communicate with the sponsors to address the potential risk of chemicals early. These help to increase the demand for safety standards. The use of the At tool in these Regulatory Reviews saves time and costs for the companies submitting new drug applications.[27]

**Role of Al in Regulatory Review:**

The AI Inclusion can greatly enhance regulatory efficiency and decision-making. And one of the key advantages of AAI is its capability to automate the data information-gaining and synthesis. This ability allows regulators to perform systematic reviews much more efficiently. The depth of this competence adds value to regulatory agencies like. [FDA]. And assisting them in remaining aware of the fast-changing scientific environment & and enhancing more evidence-based, data-driven regulatory action Artificial intelligence (AI) is increasingly shaping the field of regulatory review of drug discovery and development, offering transformative power to make evaluation processes more productive and enhance decision-making. Regulatory bodies such as the FDA, EMA, and CDSCO need to examine millions of preclinical, clinical, and post-marketing data, and AI can provide tools to improve efficiency, accuracy, and consistency. [28]Applications of AI cross a number of fields like preclinical assessment where it predicts toxicology, pharmacokinetics, and ADMET properties, clinical trial data analysis for out-of-range detection and adverse event processing, and pharmacovigilance where real-world evidence from electronic health records, social media, and spontaneous reports can be mined for safety signals. Furthermore, natural language processing (NLP) supports regulatory document management via filtering electronic Common Technical Document (eCTD) dossiers and extracting critical information from submissions and guidelines. The use of AI in these fields shortens review timelines, provides reproducible decisions, and enhances initial safety monitoring but is subject to significant challenges like reliance on high-quality standardised data, lack of transparency in black-box systems, validation limitations of outputs, and integration complications with existing regulatory frameworks. There are ethical as well as legal concerns involved, including patient data privacy under laws like GDPR and HIPAA, fairness-bias in training data that could compromise fairness, and responsibility for AI-driven regulatory decisions. To address these issues, global agencies are establishing regulatory guidelines and policies: the FDA has initiated initiatives like AI/ML for medical devices, Project PROTECT, and the Sentinel system; the EMA is encouraging regulatory science solutions for AI; and global bodies like WHO and ICH are developing harmonized digital health standards with a focus on Good Automated Manufacturing Practice (GxP) compliance and AI validation. Case studies illustrate AI's real-world use, such as the FDA's deployment of AI for pharmacovigilance, the EMA's pilot projects in clinical trial submissions, and collaborative efforts during the COVID-19 pandemic to accelerate vaccine data analysis. In the future, there is the potential to incorporate explainAble AI (XAI) to augment regulatory confidence, standardize standards between regions, apply large language models (LLMs) like GPT to regulatory insight, and develop hybrid systems with the consolidation of AI and human intuition. While beneficial challenges still await, AI holds the ability to transform regulatory review by streamlining efficiency, increasing reliability, and introducing safety, provided that industry, regulators, and AI experts collaborate to maintain responsible and transparent implementation. Toxicology prediction:The AI tool assists in studying and data collectiOn toxicology, and improves the efficiency and Accuracy.[29]

In. Statistical modeling was extensively discussed as a means to provide more detailed information. Risk characterizations are more conventional than those. It is safe or unsafe, and these AI modal tools have been

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developed for the prediction of toxicological outcomes and drug safety. Utilizing like [DL] deep learning, AI models can assist in forecasting and examining the action of chemicals (or) drugs more precisely. And the advantage of decreasing dependency on animal use. Extensibility is an advantage of At in workflow regulatory. And many of the regulation follows an Exacting & short timeline. Al can process a large volume of data quickly to study priority chemicals for further review or to communicate with the sponsors to address the potential risks of chemicals early. These help to increase the demand for safety standards. The application of the At tool in these Regulatory Reviews saves time, costs for companies that submit new drug applications.[30]

**AI in marketed product management:**

Market positioning is the activity of building an identity of the Product in the marketplace to persuade consumers to purchase them, and thus It is a vital component in nearly all business plans for companies to create their own distinct identity.[31]This strategy was employed in the promotion of pioneer drug Viagra, with the company positioning it not only for treating men's erectile dysfunction, but for a host of other issues that impact quality of life Using technology and using e-commerce as a platform, it has been made simpler for companies to achieve a natural brand recognition in the public space. Firms utilize search engines as one of the technological platforms to take a central place in Internet marketing and assist in product positioning In the marketplace, as also attested by the Internet Advertising Bureau. Firms always attempt to position their website higher than that of competing firms, providing their brand with prominence in a span of time Other methods, including statistical methods to analyze data, particle swarm optimization algorithms (introduced by Eberhart and Kennedy in 1995) coupled with NNs, gave a better insight into markets. They could assist in deciding the marketing strategy for subsequent products based on precise consumer-demand prediction.[32]

**AI in market analysis and prediction:**

The success of an organization is based on the ongoing development and enhancement of its business. Despite having access to a lot of funds, R&D yield in the pharma sector is declining due to the inability of companies to embrace new marketing technologies. The developments in digital technologies, also known as the 'Fourth Industrial Revolution assisting novel digitalized marketing through a multicriteria decision-making methodology, which aggregates and computes statisticstical and mathematical information and applies human insights to drive AI-based decision models to study innovative marketing methodology. AI also assisted in a detailed analysis of the basic needs of a product from the customer's perspective, as well as identifying the needs of the market, which supports decision-making through tools of prediction. AI can also predict sales and profile the market.[33] AI-driven software involves consumers and makes them aware among doctors by presenting ads directing the doctors to the product website with a single click. In addition, these methods use natural language-processing tools to analyze keywords entered by customers and relate them to the probability of purchasing the product. Several businesses-to-business (B2B) companies have announced self-service technologies that allow free browsing of health products, easily found by giving their specifications, placing orders, and tracking their shipping. Pharma companies are also launching their web-based applications like 1 mg, Medline, Net meds, and Ask Apollo, to meet the unserved needs of the patients Forecasting of the market is also crucial for other pharmaceutical distribution firms, which can apply AI to the domain, like 'Business intelligent Smart Sales Prediction Analysis', that employs a mixture of time series forecasting and real-time usage. This aids the pharmaceutical companies to forecast the sales of products beforehand to avoid the costs of excess stock or avoid loss of customers due to shortages[34]

**AI in product cost management:**

According to the market analysis and cost involved in the development of the pharmaceutical product, the company fixes the final Price of the product. The key idea of implementing AI to calculate this price lies in leveraging the potential of AI to mimic the thought process of an expert human in evaluating the factors that regulate a product's price once it has been manufactured. Variables, like the cost incurred in research and development of the drug, stringent price regulatory programs in the respective country, duration of the exclusivity period, market share of the innovated drug one year prior to patent expiration, reference product's price, and price-fixing policy, determine the prices of branded and generic drugs.[35] In ML, large volumes of statistical data like product development cost, product demand in the market, inventory cost, manufacturing cost, and

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competitors' product price are examined by software, later creating algorithms for the prediction of the product price. AI tools like In competitor, introduced by Intelligence Node (established in the year 2012), is a full-fledged retail competitive intelligence solution that examines the competitor price information and assists retailers and brands in tracking the competition. Wise Athena and Navetti Price Point allow the user to set the price of their product, which means pharmaceutical companies can utilize the same to aid product costing.[36]

**AI In post-market surveillance**:

It is also known as pharmacovigilance, and is increasingly important to drug safety and efficacy once products get on the market. After a drug has been licensed and used extensively, tremendous volumes of data are generated from electronic health records (EHRs), insurance claims, registries, adverse event reports, and even social media. Artificial intelligence techniques such as machine learning and natural language processing (NLP) can analyze such ginormous datasets better than can be done manually, and this results in faster detection of adverse drug reactions (ADRs), rare side effects, or safety signals that might have remained unseen during clinical trials.[37] AI also enables live monitoring through constaNot scanning health databases and patient reports enables drug regulatory agencies and pharmaceutical companies to react in real-time, such as altering safety labels, issuing warnings, or, worse, withdrawing a product from the market. AI is also supportive in detecting drug–drug interaction, patterns of misuse, or patterns of off-label use, and even detects upcoming risks in advance before they become a significant issue. By optimizing the collection, compilation, and analysis of different sources of post-marketing data, AI enhances the overall Efficiency, accuracy, and velocity of pharmacovigilance systems. However, impediments such as confidentiality of data, transparency of algorithms, and the danger of spurious signals remain, highlighting the need for explainable AI models, regulatory oversight, and industry-health authority coordination. As a whole, AI strengthens post-market surveillance by strengthening patient safety, simplifying risk identification, and easing evidence-based regulatory decision-making. N[LP] Natural language processing:[38]

**Natural Language Processing (NLP):**

It has been A strong ally in pharmacovigilance, the science of discovering, evaluating, and preventing adverse drug reactions (ADRs) and safety issues once a drug has come to market, as it allows for the effective examination of the huge quantities of unstructured text data created from spontaneous reporting systems, electronic health records (EHRs), biomedical literature, clinical notes, and even social media websites.

Historically, pharmacovigilance involved checking case safety reports and published articles by hand. Still, with the exponential growth of data, these methods have become time-consuming and error-prone, making NLP indispensable for automating and enhancing safety monitoring. NLP tools in pharmacovigilance involve retrieving drug name mentions, symptoms, and ADRs from free-text reports utilizing methods such as named entity recognition, evaluating probable causality relationships between medicines and reported effects by examining sentence grammar, identifying duplicate safety reports between databases, and reading scientific literature for pertinent safety signals and subsequently decreasing the manual workload. NLP is also at the center of social media mining, detecting early warning signals from patient-reported content, and multilingual processing to allow examination of reports received in foreign languages to aid global pharmacovigilance initiatives.[39] Methods vary from dictionary matching and rule-based systems through to more sophisticated machine learning and deep learning methodologies, with transformer models like BERT, BioBERT, and ClinicalBERT offering contextual comprehension of medical text and with integration into ontologies like MedDRA providing consistency in language. The advantages of NLP are considerable, as it provides near real-time surveillance, quicker identification of infrequent or out-of-ordinary ADRs, lower expenses, and more accurate results by reducing human mistakes in safety data curation. Yet difficulties do exist, such as vagueness in patient self-reports, noisy and incomplete social media data, challenges in translating free-text terms to standardized medical terminologies, possibilities of false positives or negatives, as well as patient privacy concerns when analyzing EHRs and online posts. Looking forward, the destiny of NLP in pharmacovigilance is the training of domain-specific large language models on pharmacovigilance datasets, integration with predictive models for evaluating ADR severity and frequency, development of real-time NLP pipelines for regulatory surveillance, improvement of explainable NLP approaches to increase trust in AI-based safety evaluation, and design of cross-lingual systems for aligning global practices of pharmacovigilance. In all, NLP is transforming

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pharmacovigilance by taking enormous volumes of unstructured safety information and turning it into usable insights, enhancing regulatory decision-making, and ultimately protecting public health[40].

## CONCLUSION:

Artificial intelligence has emerged as a transformative force in drug discovery and development, addressing long-standing challenges associated with time, cost, and attrition rates in pharmaceutical research. By enabling rapid target identification, de novo molecular design, predictive modeling, and optimization of preclinical and clinical studies, AI provides a data-driven foundation for accelerating therapeutic innovation. Integration of machine learning algorithms with omics data, molecular simulations, and real-world clinical evidence is not only enhancing precision but also uncovering novel therapeutic avenues that were previously inaccessible through Conventional methods. Despite its immense potential, AI-driven drug discovery is not without limitations, including data quality issues, interpretability of algorithms, and the need for robust regulatory frameworks to ensure safety and efficacy. Future progress will depend on collaborative efforts betComputational scientists, biologists, clinicians, and regulatory authorities need to refine methodologies, standardize validation protocols, and promote transparency in AI applications. Ultimately, AI is reshaping, the rmaceutical landscape By byidging the gap between basic research and clinical translation. With continued advancements, it promises to deliver safer, more effective, personalized therapies to patients worldwide, marking a paradigm shift in modern drug discovery and development.

## REFERENCE.


1. Ocana A, Pandiella A, Privat C, Bravo I, Luengo-Oroz M, Amir E, Gyorffy B. Integrating artificial intelligence in drug discovery and early drug development: a transformative approach. Biomarker Research. 2025 Mar 14;13(1):45.
2. Chen Y, Yang M, Hua Q. Artificial intelligence in central-peripheral interaction organ crosstalk: The future of drug discovery and clinical trials. Pharmacological Research. 2025 Apr 10:107734.
3. McGinnity DF, Meneyrol J, Boldron C, Johnstone C. Every Compound a Candidate: experience-led risk-taking approaches to accelerate small-molecule drug discovery. Drug Discovery Today. 2025 Apr 8:104354.
4. Kokudeva M, Vichev M, Naseva E, Miteva DG, Velikova T. Artificial intelligence as a tool in drug discovery and development. World Journal of Experimental Medicine. 2024 Sep 20;14(3):96042.
5. Harvey A. The role of natural products in drug discovery and development in the new millennium. I Drugs. 2010; 13:70–72. [PubMed] [Google Scholar]
6. Sivakumar B, Kaliappan I. Lead drug discovery from imidazolinone derivatives with Aurora kinase inhibitors. PHAR. 2023; 70:1529–1540. [Google Scholar]
7. Kumar V, Roy K. Embracing the changes and challenges with modern early drug discovery. Expert Opinion on Drug Discovery. 2025 Apr 3;20(4):419-31.
8. Garg P, Singhal G, Kulkarni P, Horne D, Salgia R, Singhal SS. Artificial intelligence–driven computational approaches in the development of anticancer drugs. Cancers. 2024 Nov 20;16(22):3884.
9. Varg P, Singhal G, Kulkarni P, Horne D, Salgia R, Singhal SS. Artificial intelligence–driven computational approaches in the development of anticancer drugs. Cancers. 2024 Nov 20;16(22):3884
10. Garg P, Singhal G, Kulkarni P, Horne D, Salgia R, Singhal SS. Artificial intelligence–driven computational approaches in the development of anticancer drugs. Cancers. 2024 Nov 20;16(22):3884.
11. Jarallah SJ, Almughem FA, Alhumaid NK, Fayez NA, Alradwan I, Alsulami KA, Tawfik EA, Alshehri AA. Artificial intelligence revolution in drug discovery: A paradigm shifts in pharmaceutical innovation. International Journal of Pharmaceutics. 2025 May 30:125789.
12. Rotake SB, Hatwar PR, Bakal RL, Meshram SI. The role of Artificial Intelligence in drug discovery. Journal of Drug Delivery & Therapeutics. 2025 Jul 1;15(7).
13. Patel V, Shah M. Artificial intelligence and machine learning in drug discovery and development. Intelligent Medicine. 2022 Aug 1;2(3):134-40.
14. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug discovery today. 2019 Mar 1;24(3):773-80.
15. Agrawal P. Artificial intelligence in drug discovery and development. Journal of Pharmacovigilance. 2018;6(2):1000e173.

16. Chen W, Liu X, Zhang S, Chen S. Artificial intelligence for drug discovery: Resources, methods, and applications. Molecular therapy Nucleic acids. 2023 Mar 14; 31:691-702.
17. Ocana A, Pandiella A, Privat C, Bravo I, Luengo-Oroz M, Amir E, Gyorffy B. Integrating artificial intelligence in drug discovery and early drug development: a transformative approach. Biomarker Research. 2025 Mar 14;13(1):45.
18. Bassey GE, Daniel EA, Okesina KB, Odetayo AF. Transformative Role of Artificial Intelligence in Drug Discovery and Translational Medicine: Innovations, Challenges, and Future Prospects. Drug Design, Development and Therapy. 2025 Dec 31:7493-502.
19. Sulahian R, et al. Synthetic lethal interaction of SHOC2 depletion with MEK Inhibition in RAS-Driven cancers. Cell Rep. 2019; 29:118–e1348.
20. Kryukov GV, et al. MTAP deletion confers enhanced dependency on the PRMT5 arginine methyltransferase in cancer cells. Science. 2016; 351:1214–8.
21. Imming P, Sinning C, Meyer A. Drugs, their targets and the nature and number of drug targets. Nat Rev Drug Discov. 2006; 5:821–34.
22. Ocana A, Pandiella A, Privat C, Bravo I, Luengo-Oroz M, Amir E, Gyorffy B. Integrating artificial intelligence in drug discovery and early drug development: a transformative approach. Biomarker Research. 2025 Mar 14;13(1):45.
23. Akhtar M, Nehal N, Gull A, Parveen R, Khan S, Khan S, Ali J. Explicating the transformative role of artificial intelligence in designing targeted nanomedicine. Expert Opinion on Drug Delivery. 2025 May 23:1-21.
24. Shalem O, Sanjana NE, Zhang F. High-throughput functional genomics using CRISPR–Cas9. Nat Rev Genet. 2015;16:299–311.
25. Wang T, et al. Identification and characterization of essential genes in the human genome. Science. 2015; 350:1096–101.
26. Rask-Andersen M, Almén MS, Schiöth HB. Trends in the exploitation of novel drug targets. Nat Rev Drug Discov. 2011; 10:579–90.
27. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. Drug discovery today. 2019 Mar 1;24(3):773-80.
28. Sankar R, Alam MN. Artificial Intelligence in Drug Development and Delivery: Opportunities, Challenges, and Future Directions. Journal of Angiotherapy. 2024 Aug 9;8(8):1-0.
29. Al Kuwaiti A, Nazer K, Al-Reedy A, Al-Shehri S, Al-Muhanna A, Subbarayalu AV, Al Muhanna D, Al-Muhanna FA. A review of the role of artificial intelligence in healthcare. Journal of personalized medicine. 2023 Jun 5;13(6):951.
30. Vora LK, Gholap AD, Jetha K, Thakur RR, Solanki HK, Chavda VP. Artificial intelligence in pharmaceutical technology and drug delivery design. Pharmaceutics. 2023 Jul 10;15(7):1916.
31. Blanco-Gonzalez A, Cabezon A, Seco-Gonzalez A, Conde-Torres D, Antelo-Riveiro P, Pineiro A, Garcia-Fandino R. The role of AI in drug discovery: challenges, opportunities, and strategies. Pharmaceuticals. 2023 Jun 18;16(6):891.
32. Sarkar C, Das B, Rawat VS, Wahlang JB, Nongpiur A, Tiewsoh I, Lyngdoh NM, Das D, Bidarolli M, Sony HT. Artificial intelligence and machine learning technology driven modern drug discovery and development. International Journal of Molecular Sciences. 2023 Jan 19;24(3):2026.
33. Sarkar C, Das B, Rawat VS, Wahlang JB, Nongpiur A, Tiewsoh I, Lyngdoh NM, Das D, Bidarolli M, Sony HT. Artificial intelligence and machine learning technology driven modern drug discovery and development. International Journal of Molecular Sciences. 2023 Jan 19;24(3):2026.
34. Xiao, X.; Min, J.L.; Lin, W.Z.; Liu, Z.; Cheng, X.; Chou, K.C. I Drug-Target: Predicting the interactions between drug compounds and target proteins in cellular networking via benchmark dataset optimization approach. J. Biomol. Struct. Dyn. **2015**, 33, 2221–2233. [**Google Scholar**] [**CrossRef**]
35. Koromina, M.; Pandi, M.T.; Patrinos, G.P. Rethinking drug repositioning and development with artificial intelligence, machine learning, and omics. Omics **2019**, 23, 539–548. [**Google Scholar**] [**CrossRef**]
36. Segler, M.H.S.; Kogej, T.; Tyrchan, C.; Waller, M.P. Generating Focused Molecule Libraries for Drug Discovery with Recurrent Neural Networks. ACS Cent. Sci. **2017**, 4, 120–131. [**Google Scholar**] [**CrossRef**]
37. Kim, K.H.; Kim, N.D.; Seong, B.L. Pharmacophore-based virtual screening: A review of recent applications. Expert Opin. Drug Discov. **2010**, 5, 205–222. [**Google Scholar**] [**CrossRef**]

ISSN No. 2321-2705 | DOI: 10.51244/IJRSI |Volume XII Issue X October 2025

38. Serrano DR, Luciano FC, Anaya BJ, Ongoren B, Kara A, Molina G, Ramirez BI, Sánchez-Guirales SA, Simon JA, Tomietto G, Rapti C. Artificial intelligence (AI) applications in drug discovery and drug delivery: Revolutionizing personalized medicine. Pharmaceutics. 2024 Oct 14;16(10):1328.
39. Obaido G, Mienye ID, Egbelowo OF, Emmanuel ID, Ogunleye A, Ogbuokiri B, Mienye P, Aruleba K. Supervised machine learning in drug discovery and development: Algorithms, applications, challenges, and prospects. Machine Learning with Applications. 2024 Sep 1; 17:100576.
40. Xiao W, Jiang W, Chen Z, Huang Y, Mao J, Zheng W, Hu Y, Shi J. Advance in peptide-based drug development: delivery platforms, therapeutics and vaccines. Signal Transduction and Targeted Therapy. 2025 Mar 5;10(1):74.