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Revolutionizing Drug Discovery With AI From Target Identification To Post-Marketing Surveillance

Abstract

Background: Artificial Intelligence (AI) is transforming drug discovery by enhancing efficiency, accuracy, and cost-effectiveness across the entire development pipeline, from target identification to post-marketing surveillance. Since its origins in the 1950s, AI has evolved into a vital tool in pharmaceuticals. Technologies such as Machine Learning (ML) and Deep Learning (DL) have improved our understanding of disease mechanisms, pharmacokinetics, and clinical trial design.

Methodology: This review examines AI applications across four major stages of drug discovery: target identification, preclinical development, clinical trials, and post-marketing surveillance. Insights and regulatory perspectives from agencies such as the US FDA, EMA, Health Canada, and other ethical and regulatory bodies are also discussed.

Results: AI significantly accelerates drug discovery by rapidly identifying potential targets, predicting ADMET properties, and optimising clinical trial design. It also strengthens post-marketing surveillance through early detection of safety signals. These advancements collectively improve precision, reduce development timelines, and enhance drug safety and efficacy.

Conclusion: AI is revolutionising drug discovery by streamlining processes from early target identification to post-approval monitoring. Its ability to support virtual screening, improve drug design, and enhance decision-making is expected to lead to safer and more effective therapies, ultimately advancing patient outcomes and innovation in the pharmaceutical industry.

INTRODUCTION

Artificial intelligence (AI) is rapidly reshaping drug discovery by enhancing the efficiency, accuracy, and cost-effectiveness of processes across the development pipeline. With the ability to analyze complex biological data, predict molecular interactions, and support informed decision-making, AI has become an essential tool in modern pharmaceutical research. Its applications now span target identification, virtual screening, drug design, pharmacokinetic prediction, clinical trial optimization, and post-marketing safety monitoring.

Given the increasing integration of AI into drug development, there is a growing need to understand its role, benefits, and regulatory implications. This review aims to provide a comprehensive overview of how AI contributes to the major stages of drug discovery, including target identification, preclinical assessment, clinical research, and post-market surveillance. It also evaluates the perspectives of key regulatory authorities such as the US FDA, EMA, and Health Canada, highlighting the challenges and expectations associated with AI-driven tools in pharmaceuticals.

By examining both scientific applications and regulatory considerations, this review outlines the current landscape of AI in drug discovery and emphasizes its potential to support faster, more precise, and safer therapeutic development.

Discussion

Target Identification

AI-powered target identification in drug discovery combines computational, multi-omics, and experimental methods to improve efficiency and precision in identifying therapeutic targets such as proteins, genes, and RNA. Computational techniques, such as AI-driven algorithms and structure-based methods like reverse docking and pharmacophore screening, use large datasets to analyze molecular interactions and predict novel targets. Multi-omics data, which includes genomics, transcriptomics, proteomics, metabolomics, and epigenomics, provide a comprehensive understanding of biological processes, allowing for the identification of complex disease mechanisms and potential targets. Experimental approaches, such as affinity-based techniques, chemical-genetic strategies (e.g., CRISPR/Cas9), and comparative profiling (e.g., SILAC), supplement AI by validating targets through functional and phenotypic research. AI and these methodologies work together to revolutionize target identification, accelerating the development of personalized and effective therapies by generating novel therapeutic hypotheses and increasing our understanding of complex diseases.2 This is illustrated in Figure No.01.

AI analyzes large amounts of biological and chemical data to identify the most promising drug candidates. Machine learning algorithms can predict a drug's toxicity, metabolism, bioavailability, and possible side effects before laboratory or animal testing. This helps researchers eliminate unsuitable compounds at an early stage, saving time and resources.

AI also predicts drug-target interactions and identifies disease biomarkers, helping scientists understand disease mechanisms and develop better therapies. Deep learning models analyze images from cell cultures, tissues, and animal studies quickly and accurately, reducing manual errors.

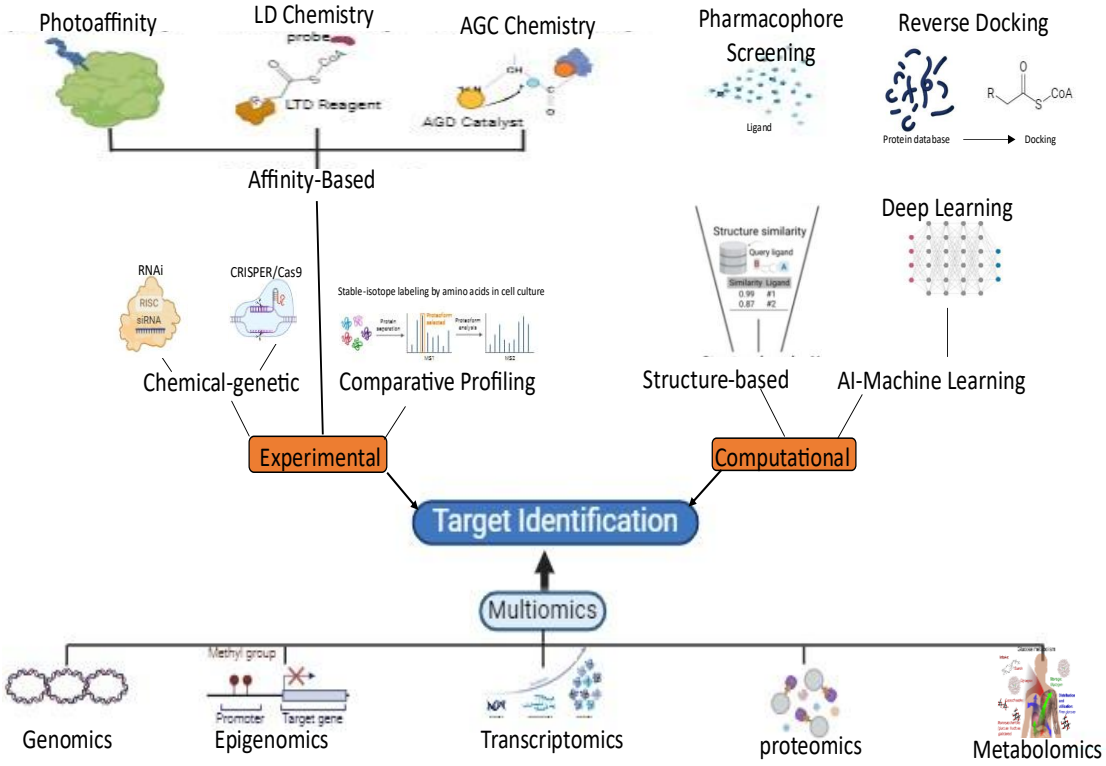

Figure 1:Target Identification in Drug Discovery in AI

AI in Virtual Screening

AI in Virtual Screening uses various search algorithms, including Monte Carlo, genetic algorithms, and systematic search. The Monte Carlo method randomly tests various possible molecules to determine which ones perform best. Genetic algorithms mimic natural selection by iterating and improving drug candidates. Systematic search thoroughly examines every possible drug molecule, without skipping any options.

Databases are critical for AI-powered virtual screening because they provide the data required for predictions. For example, PDBBind contains detailed information on molecule-protein interactions, whereas ChEMBL and PubChem provide large collections of chemical data that AI can use to better understand the properties of various molecules. AI virtual screening can be structure-based, where AI analyzes the 3D structure of a target protein, or ligand-based, where AI looks for molecules that share similarities with known drug-like molecules3. This was shown in Figure 2

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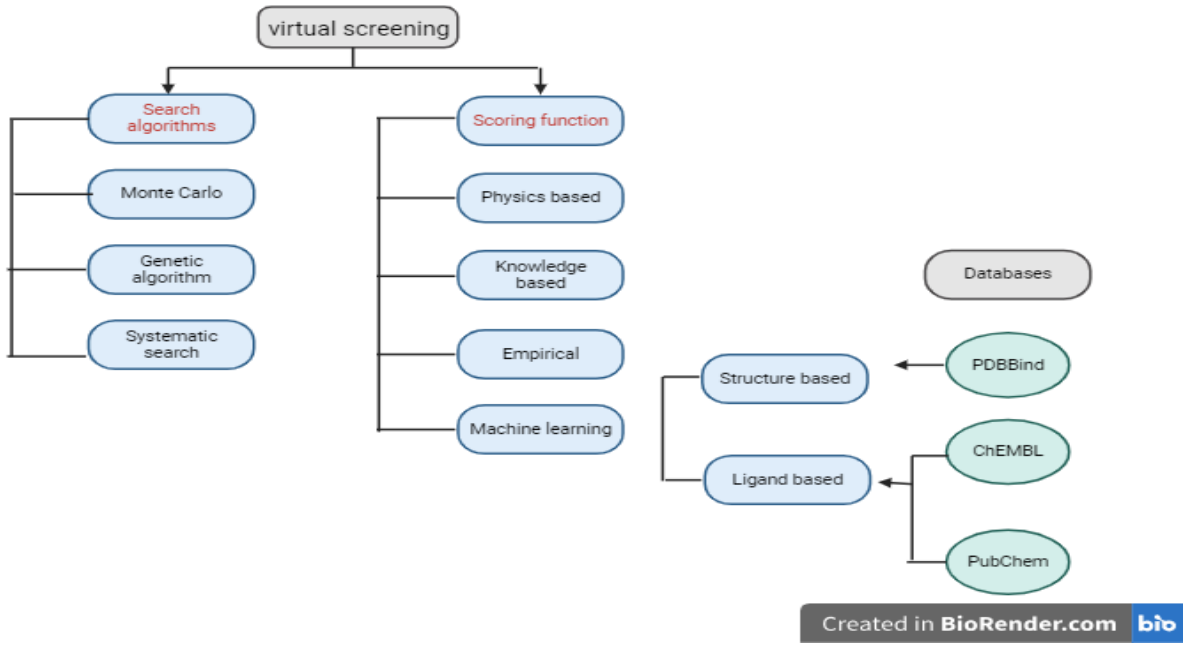

Figure 2: Two main components of virtual screening (VS) and different types of scoring functions. Machine learning (ML) scoring functions are classified as ligand-based (or descriptor-based) and structure-based depending upon the use of descriptors for ligands alone or for both target and ligands.

Machine learning (ML) models aid in drug discovery by analyzing data on protein-drug interactions. These models go through three major stages: training, testing, and validation, with validation often performed using separate data. Once validated, these models can search large chemical libraries, such as ZINC or DrugBank, for potential new drugs.

However, the drug compounds identified by these models are rarely experimentally tested in labs because the process involves challenges such as synthesis or purchasing the compounds for further biological testing. Despite these challenges, some ML and deep learning (DL) models have been experimentally validated, which is critical for establishing trust in using AI for drug discovery. The section highlights success stories where AI-based models have been tested in real-life lab experiments and provides4 a list of these examples in Table 1.

Ligand-based deep learning and machine learning Models:

A study on predicting inhibitors of the CYP1A2 enzyme demonstrates how machine learning can help identify potential drug candidates. Researchers looked through a database of 16,338 compounds and tested 41 for CYP1A2 inhibition. Six of the 19 compounds selected using a Random Forest (RF) approach were effective, with IC50 values (a measure of potency) ranging from 48 to 231 nM. Meanwhile, compounds discovered using docking methods demonstrated greater potency but less chemical diversity. While docking yielded more potent inhibitors, ML-based methods proved to be more efficient and effective for early drug discovery.

In another example, ML models such as DNN (Deep Neural Network) and RF were used to identify inhibitors of triple-negative breast cancer (TNBC) and m-opioid receptors. These models outperformed traditional methods, identifying several promising compounds with high inhibitory potential.

Various machine learning models, including Random Forest, XGBoost, and others, have been used to screen compound libraries for cancer, Alzheimer's, and infectious diseases.

Table 1:Summary of Machine Learning and Deep Learning-Based Virtual Screening Studies for Hit Identification

Summary of hit identification from virtual screening studies using machine and deep learning approaches					
Method LBML(Ligand-Based Machine Learning)	**Target**	**Hits**	**Activity(IC_{50})**	**Year**	**Refs**
P-SAMPNN	Anti-osteoclastogenesis-a process that breaks down bone tissue	2	32-68 nM	2021	
RF/DNN	Aryl hydrocarbon receptor-a protein that affects responses to toxins	45	NA	2021	
XGBoost	OCT 1inhibitors-The focus was on identifying inhibitors of **OCT1**, a transporter protein that helps move drugs into cells.	16	Mean Km 127±50mM	2021	
NB	GSK3α and GSKβ-It are involved in several diseases like diabetes and cancer.	2	GSK3β=97.3 Nm;GSK3α=695.9 nM	2020	
DNN/RF	Triple-negative breast cancer inhibition-find drugs that inhibit **triple-negative breast cancer**, a difficult-to-treat type of cancer.	4	1.49-10.7 mM	2020	
DNN/RF	m-opioid receptor agonists	5	EC_{50} 0.56-8.05 mM	2020	
RF/GCNN	Multitargets	6	1-21nM	2020	
SVM	FGFR4 and EGFR	1	FGFR4=86.2 Nm;EGFR=83.9 nM	2020	

AI in Drug Design

Target identification (1-2 years) is the first step in the drug design and development process. Using methods like protein-protein interaction (PPI) prediction and de novo drug design, researchers find and validate biological targets, such as proteins connected to a particular disease. Because it creates the foundation for the entire development process, this step is crucial. Then, over the course of Hit Discovery (one to two years), a large number of compounds are screened using techniques like pharmacophore modeling, QSAR modeling, and high-throughput virtual screening (HTVS) to find "hits" that interact with the identified target, thereby reducing the number of possible drug candidates from vast chemical libraries. Following the discovery of hits, researchers alter the chemical structures of these hits to increase their efficacy during the Lead Optimization phase, which lasts one to three years, usually involving several rounds of synthesis and testing. After optimization, the drug enters the Preclinical Stage (1-2 years), during which it is tested in animal models to determine its safety, toxicity, pharmacokinetics (how it behaves in the body), and pharmacodynamics (its effects on the body), as well as biomarker assessments to better understand its mechanism of action. Clinical trials (5-7 years) are the next step, divided into phases I, II, and III, in which the drug is tested on humans to determine its safety and effectiveness. This is the longest and most expensive stage, with AI used in personalized medicine and data analysis to tailor treatments to individual patients for best results. Following successful clinical trials, the drug developer submits a New Drug Application (NDA) for regulatory approval, after which all previous data is rigorously reviewed. Once approved, the drug is cleared for marketing and distribution, allowing patients to receive treatment5. This was illustrated in Figure No. 3.

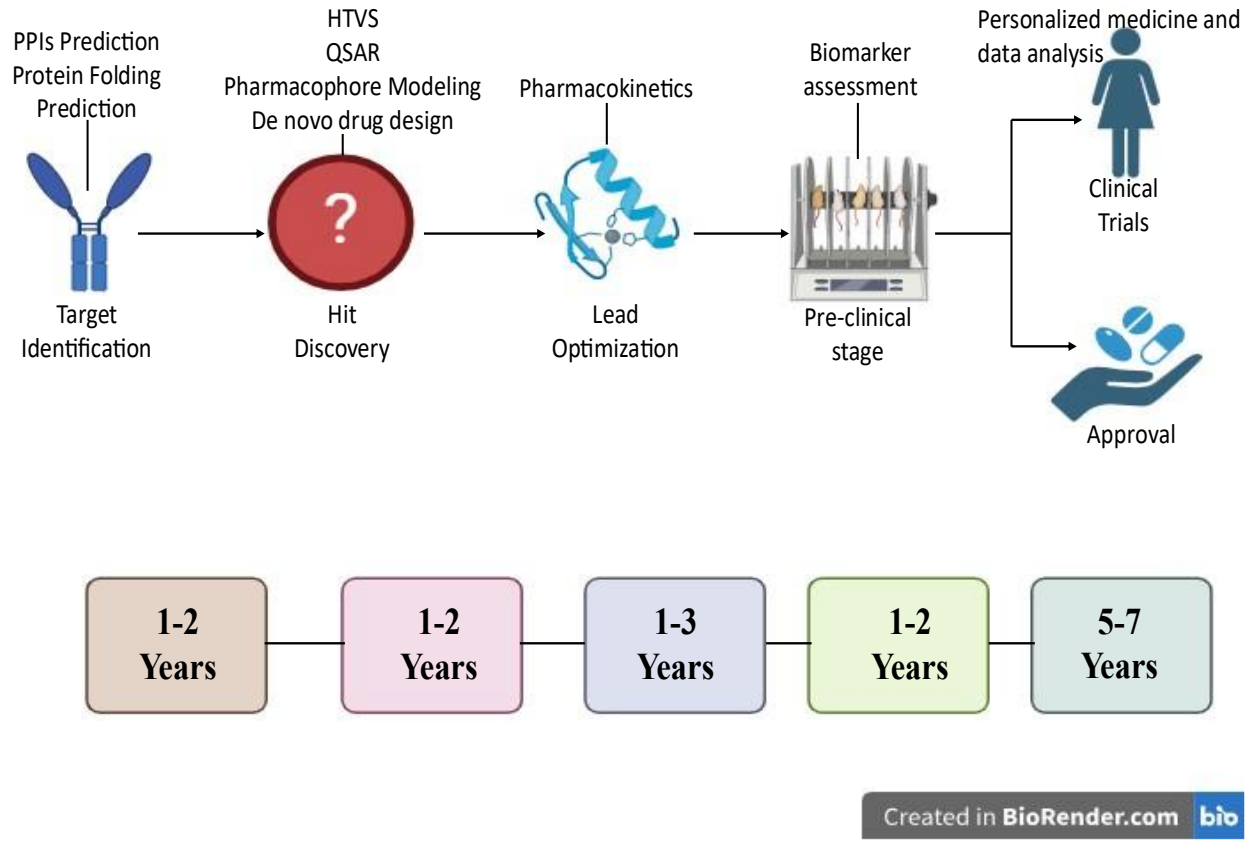

Figure 3:overview of drug design and development process, and the implementation in artificial intelligence in various fields

Table 2: Applications of Artificial Intelligence in Drug Formulation and Development

Sl. No.	Application	Role of AI
1	Excipient Selection	AI predicts the most suitable excipients based on the drug's physical and chemical properties.
2	Formulation Optimization	Machine learning identifies the optimal composition of APIs and excipients to achieve desired characteristics such as dissolution, stability, and bioavailability.
3	Stability Prediction	AI models estimate shelf life and predict drug degradation under different storage conditions, reducing the need for lengthy stability studies.
4	Solubility Enhancement	AI recommends techniques such as solid dispersions, nanoparticles, lipid-based systems, or cyclodextrin complexes to improve poorly soluble drugs.
5	Controlled and Sustained Release	AI helps design formulations that release the drug at a specific rate and duration.
6	Quality by Design (QbD)	AI analyzes process parameters and critical quality attributes to optimize manufacturing and ensure consistent product quality.
7	Process Optimization	AI supports manufacturing by optimizing mixing, granulation, compression, coating, and other production steps.
8	Personalized Medicine	AI enables the design of patient-specific formulations based on factors such as age, genetics, disease state, and therapeutic needs.

AI in Pre-Clinical Development

Artificial Intelligence (AI), along with Machine Learning (ML) and Deep Learning (DL), is revolutionizing drug discovery, particularly in the preclinical stage. AI is a powerful tool for predicting key properties of drug molecules such as absorption, distribution, metabolism, and potential toxicity, all of which are important for drug safety and efficacy. AI models learn from massive amounts of data, making it possible to create new drugs more efficiently. Different types of machine learning, such as supervised learning, help predict specific drug-target interactions, whereas unsupervised learning looks for patterns in chemical compounds. Reinforcement learning, while still experimental, allows artificial intelligence to improve drug design through trial and error.

Deep Learning (DL), a more advanced subset of ML, employs neural networks to handle complex, unstructured data such as 3D molecular structures. Convolutional Neural Networks (CNNs), a type of deep learning, are particularly useful for analysing how small drug molecules bind to proteins, which is an important step in drug discovery. AI, ML, and DL speed up various stages of drug development, from predicting drug behaviour in

the body to identifying the most promising compounds for future research. These technologies not only speed up the drug discovery process but also lower costs and improve the accuracy of identifying potential drug candidates. In Figure 4

AI finds the most promising medicine candidates by analysing vast volumes of chemical and biological data. Prior to laboratory or animal testing, machine learning algorithms can forecast a drug's toxicity, metabolism, bioavailability, and potential adverse effects. This saves time and money by assisting researchers in the early removal of inappropriate chemicals

Additionally, AI finds disease biomarkers and forecasts drug-target interactions, assisting researchers in comprehending disease causes and creating more effective treatments. Deep learning algorithms reduce human error by rapidly and reliably analysing images from animal studies, tissues, and cell cultures.

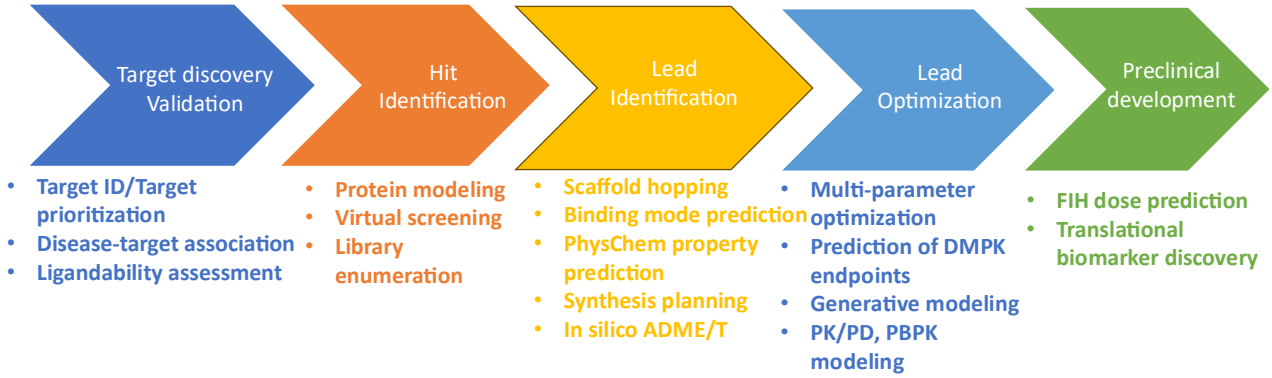

Figure 4: opportunities for the application of AI technique in drug discovery.schematic representation of the pre-clinical drug discovery process highlighting opportunities for AI to be applied across drug discovery continuum

AI, Machine Learning (ML), and Deep Learning (DL) are critical in the preclinical phase of drug discovery because they improve the efficiency and accuracy of key processes such as lead optimization, ADMET prediction, and complex data analysis such as 3D molecular structures. Supervised and unsupervised machine learning algorithms help predict drug behavior and group similar compounds, whereas reinforcement learning (RL) aids in the design of molecules with desirable properties. DL techniques, such as Convolutional Neural Networks (CNNs), are particularly useful for modeling protein-ligand interactions, which are critical to understanding drug efficacy. AI accelerates the preclinical phase by streamlining data analysis and reducing the number of physical tests required, lowering costs and increasing the likelihood of moving promising drug candidates to clinical trials6.FIG 5

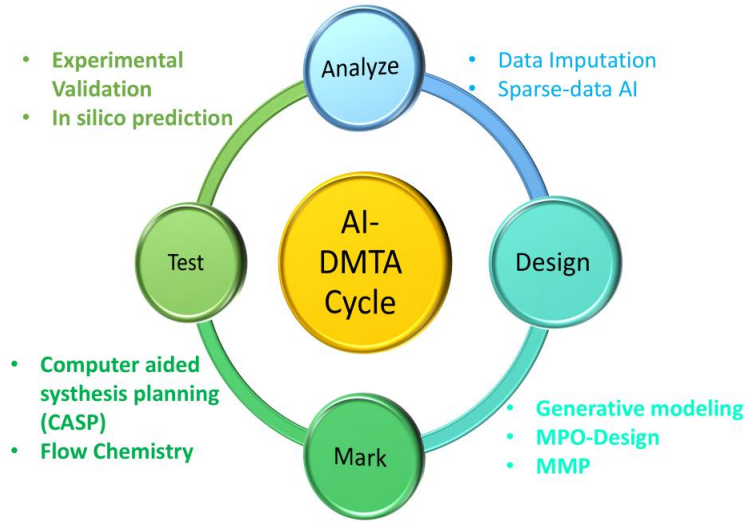

Figure 5: AI-driven design-make-test-analyze cycle highlighting opportunities to leverage Ai to increase the effectiveness of the DMTA cycle.

In preclinical drug discovery, the goal is to find potential drug candidates that can interact with biological targets (usually proteins) involved in diseases. The structural information of these targets and advances in artificial intelligence (AI) are crucial for guiding the discovery process in several stages, improving the efficiency and accuracy of identifying new drugs. Here's a detailed explanation of how structural enablement and AI accelerate.Artificial Neural Networks (ANNs), often integrated with fuzzy logic models, are extensively used

to optimize tablet manufacturing. These systems analyze the relationship between machine operating parameters and manufacturing defects such as tablet capping. By identifying optimal machine settings, AI reduces production defects, improves tablet quality, and minimizes manufacturing losses.

AI also plays a crucial role in quality assurance and quality control. Intelligent systems such as Meta-Classifier and Tablet-Classifier automatically inspect manufactured tablets, detect defects, and identify deviations from predefined quality standards. These tools enable rapid, real-time quality assessment, ensuring consistent product quality while reducing manual inspection efforts.

Furthermore, AI supports the advancement of personalized medicine through intelligent dosage design. AI-based systems have been developed that analyze patient-specific clinical information and determine the most appropriate drug combinations and dosage regimens. Such systems can also design customized transdermal patches tailored to individual patient needs, paving the way for precision pharmaceutical manufacturing.

Overall, AI has become an integral component of modern pharmaceutical manufacturing by enabling process automation, predictive modeling, intelligent quality control, equipment optimization, and personalized drug production. These technologies enhance manufacturing efficiency, reduce operational costs, improve product quality, and support the development of next-generation smart pharmaceutical production systems.

drug discovery

1. Target Identification and Validation:

- Proteins implicated in disease processes are commonly drug targets. Because it enables researchers to identify the precise areas (active sites or pockets) where a drug can bind, an understanding of the three-dimensional structure of these proteins is essential7.

2. Hit Identification Using Virtual Screening (VS):

- Structure-based virtual screening (SBVS) is a common term for this.
- AI algorithms play an important role in this process. They can simulate the interaction of millions of compounds with the target's binding site, allowing for the rapid identification of hit molecules—those with the potential to bind to the target effectively.
- AI tool, compares a target's binding site to known binding sites of other proteins using 3D representations. This helps determine whether a compound that binds to one protein will also bind to another (potentially predicting off-target effects or opportunities for drug repurposing)8.

3. Fragment-Based Drug Discovery (FBDD):

- Fragment-based drug discovery involves screening small molecular fragments that can bind to the target protein in specific locations but are too small to be drugs. Once these fragments have been identified, they can be chemically combined or grown to form larger molecules (drug candidates) with better binding properties.
- AI-predicted or experimentally derived protein structures provide structural insights that aid in designing and optimizing fragment interactions for better binding. This leads to the development of molecules with greater affinity and specificity for the target9.

4. Lead Optimization via Structure-Based Drug Design (SBDD):

- After identifying hits or fragments, researchers refine the drug's structure to improve binding affinity, efficacy, and selectivity (lead optimization).
- Structure-based drug design (SBDD) relies on detailed information about drug-target interactions to guide the design process. Researchers can visualize how a drug binds to a target and then modify its chemical structure to improve its efficacy or minimize side effects.
- Deep learning AI models can predict drug interactions with targets, speeding up the optimization process. AI can also help predict potential issues such as drug resistance10.

5. Selectivity and Off-Target Effects:

- Selective drug discovery involves avoiding off-target binding, which can lead to side effects.
- AI can compare the target protein's binding sites to other proteins in the human proteome. DeeplyTough, for example, allows you to compare binding pockets across different proteins. This allows researchers to predict whether a drug will unintentionally bind to another protein and cause off-target effects, improving safety profiles prior to clinical trials11.

6. Allosteric Sites and Resistance Mechanisms:

- Allosteric sites are regions of the protein that, when bound by a drug, can alter the activity of the protein even though the drug doesn't bind to the main active site. These sites are often harder to identify through traditional methods.
- Structural information, combined with AI algorithms, can reveal these hidden allosteric sites, which can then be targeted for drug development. Targeting allosteric sites can sometimes overcome drug resistance mechanisms, where mutations in the active site prevent drugs from binding effectively12.

7. De Novo Drug Design and AI's Role in Protein Folding:

- AI is also involved in de novo drug design, where completely new drug molecules are designed from scratch. AI algorithms can predict how a new molecule will fold and interact with the target protein, even if there is no pre-existing molecule to start with.
- Advances in AI, particularly AlphaFold2 and similar models, have greatly enhanced our ability to predict protein folding—the process by which a protein takes its 3D shape, which is

crucial for its function. Accurately predicting protein folds allows researchers to design drugs that precisely fit the target protein's structure, leading to more effective therapies13.

8. AI in Protein Structure and Folding:

- AlphaFold2 and other deep learning-based algorithms have revolutionized the ability to predict 3D structures, without needing experimental data. These predicted structures are now being used in preclinical drug discovery to fill the gaps where no experimental structures exist.
- The accuracy of AI-predicted structures allows drug developers to move forward with SBDD and FBDD approaches even in cases where structural data for the target is unavailable, greatly accelerating the drug discovery timeline14.

9. Accelerating Drug Discovery Pipelines:

- By integrating structural biology with AI, preclinical research is faster, more efficient, and cost-effective. AI-powered tools can predict protein structures, model drug-target interactions, and suggest optimizations, all while minimizing the need for labor-intensive experimental techniques.
- The ability to compare thousands of potential drug-target interactions in silico (using computational methods) dramatically reduces the number of molecules that need to be tested experimentally, focusing efforts on the most promising candidates15.

Table 3: Applications of Artificial Intelligence in Pharmaceutical Drug Characterization and Analysis

Sl. No.	Area	AI Applications	Properties / Parameters Assessed	Common AI Methods / Techniques
1	Predicting Physicochemical Properties	AI models estimate important drug properties before synthesis.	• Solubility• Lipophilicity (LogP/LogD)• pKa• Melting point• Permeability• Chemical stability	• Random Forest• Gradient Boosting• Deep Neural Networks• Graph Neural Networks (GNNs)
2	Protein and Biologic Characterization	AI analyzes characteristics of biologic drugs such as monoclonal antibodies.	• Glycosylation patterns• Protein folding• Aggregation• Post-translational modifications• Protein stability	AI/ML-based protein analysis and prediction models
3	Structure Characterization	AI assists in determining molecular structures from analytical data.	• Mass spectrometry spectra interpretation• NMR spectra prediction• Protein structure prediction• Identification of unknown impurities	AI-based spectral analysis and structure prediction models
4	Image-Based Characterization	Deep learning analyzes microscopy images for characterization of pharmaceutical materials.	• Crystal morphology• Particle size• Cell morphology• Protein aggregation• Nanoparticle characteristics	• Convolutional Neural Networks (CNNs)• Vision Transformers (ViTs)
5	Chromatography Analysis	AI automates the interpretation of chromatographic data such as HPLC, GC, and LC-MS.	• Peak detection• Impurity classification• Retention time prediction• Anomalous batch identification	AI/ML-based chromatographic data analysis

AI in ADMET

Today, AI models such as multitask deep neural networks (DNNs) can predict these properties early on, improving accuracy and lowering drug failure rates. Furthermore, AI automates Matched Molecular Pair (MMP) analysis, which detects minor structural changes in molecules to optimize their ADMET profiles. In synthesis, AI-powered Computer-Aided Synthesis Planning (CASP) helps researchers plan how to make drugs in the lab using both rule-based and template-free approaches. This increases the efficiency of synthesis routes while reducing failures. Despite these advances, challenges such as predicting stereochemistry and reaction conditions remain to be addressed. Overall, artificial intelligence is significantly accelerating and improving the drug discovery process.

In drug development, Understanding how a drug interacts with the body starts with absorption. Caco-2 permeability determines how well a drug passes through intestinal cells, whereas the Caco-2 efflux ratio predicts whether the drug will be actively pushed out of cells, affecting overall absorption. PAMPA permeability assesses a drug's ability to pass through membranes and provides insights into passive diffusion. Drugs targeting the brain are also tested for blood-brain barrier penetration to ensure they can effectively reach the brain, though this may be undesirable for some drugs.

The distribution of a drug in the body begins after it has been absorbed. Human serum albumin binding and plasma-protein binding influence how much of the drug is bound to proteins in the blood, which can reduce its activity because only unbound drugs can exert their effects. The fraction unbound (fu) indicates how much of the drug is still free in the bloodstream, whereas the volume of distribution (vdss) measures how widely the drug spreads throughout the body's tissues. For drugs that

target the central nervous system, the brain/plasma ratio (Kp) indicates how the drug is distributed between the brain and the blood.

Next, drug metabolism has a significant impact on its efficacy and safety. Microsomal and hepatocyte stability assess how quickly a drug is broken down in the liver, with unstable drugs metabolized too quickly to be effective. The site of metabolism determines where this breakdown occurs, which aids in predicting interactions and side effects. Excretion is closely related to metabolism, with CLint (intrinsic clearance) determining how well the liver clears the drug and the terminal half-life indicating how long the drug remains active in the body.

Drug behavior is influenced by physicochemical characteristics like pKa, membrane affinity, logD, and aqueous solubility.These properties influence how the drug dissolves, passes through cell membranes, interacts with tissues, and maintains the balance of water and fat environments in the body16. This is illustrated in Table 4

Table 4:Comprehensive Overview of ADMET and Physicochemical Parameters Used in Drug Discovery

Caco-2 permeability	Human serum albumin binding	Microsomal stability	CLint	Ames mutagenicity	Aq. solubility
Caco-2 efflux ratio	Plasma-protein binding	Hepatocyte stability	Terminal half-life	CYP inhibition	LogD
PAMPA permeability	Fraction unbound (fu)	Site of metabolism		Phaspholipidosis	Membrane affinity
Blood-brain barrier penetration	Volume of distribution (vdss)			hERG inhibition	pka
	Brain/plasma ratio (Kp)			Drug-induced liver injury (DILI)	

AI in Clinical Trials

AI is revolutionizing drug discovery by automating many of the most time-consuming processes. This allows for a much larger scale of exploration and faster results. For example, knowledge graphs analyze massive datasets (like OMICS data) to uncover insights into disease biology, helping researchers identify new drug targets and biomarkers. Generative AI is used to design new small molecules, while tools like AlphaFold predict how proteins fold, which is essential for designing antibodies and other protein-based drugs. Additionally, AI can repurpose existing drugs by discovering new uses for them, significantly speeding up the development of treatments.

Over the last decade, AI discovered drug and vaccine molecules, with small molecules discovered using AI now matching those discovered using traditional methods. This trend continues, with AI accelerating the discovery of biologics, albeit at a slower rate. By early 2024, all top 20 pharmaceutical companies had embraced AI in their research, frequently partnering with AI-focused biotech firms, and increasing collaborations. Despite this progress, questions remain about the quality, safety, and clinical efficacy of AI-discovered drugs. A preliminary analysis has begun to address these concerns, but more research is required as the field rapidly evolves.

AI in clinical trials is based on data from AI-native biotech companies, which account for a significant portion of AI-driven drug discovery. By reviewing pipeline data from over 100 companies, the study identified 75 AI-discovered molecules that have entered clinical trials since 2015, with 67 still in progress as of 2023. The majority of these molecules are in Phase I, with a strong emphasis on oncology (50% in Phases I and II). AI-discovered small molecules accounting for more than 30%. Vaccines and antibodies have smaller shares (10% and 5%, respectively).

Clinical success rates for AI-discovered molecules were promising, with 80-90% of molecules successfully completing Phase I trials, far exceeding the historical industry average of 40-55%. In Phase II, the success rate was around 40%, which is consistent with traditional success rates. However, the sample size is small, and the analysis only includes AI-native biotech companies and their pharma partners, leaving out AI-discovered molecules from larger pharmaceutical companies. These success rates may change as new data becomes available.

The study concludes that AI-powered drug discovery is showing great promise, particularly in early-stage clinical trials. AI-discovered molecules in Phase I trials have achieved a success rate of 80-90%, which is significantly higher than the historical average of 40-55%. This higher success rate could be due to a variety of factors. One possible explanation is that AI algorithms target well-validated biological pathways, lowering the likelihood of toxicity. However, early indications suggest that AI is also successful in identifying novel targets, as evidenced by several molecules that passed Phase I trials despite being based on previously unknown targets.

AI-discovered Phase II has a success rate of 40% when the focus shifts to proving biological efficacy, which is

consistent with traditional industry averages. This phase is more difficult because it evaluates the therapeutic concept in a clinical setting, and many AI-designed molecules must still demonstrate efficacy. a small percentage of the molecules discontinued after Phase II failed due to poor trial results.

Overall, AI has significant potential in drug discovery, particularly for increasing success rates in early-stage clinical trials. However, clinical efficacy remains a significant challenge, and as AI-driven molecules progress through later stages of development, more data will be required to fully understand these technologies' long-term success. The findings also show that AI is pushing the boundaries of novel molecule discovery, potentially reshaping the future of drug development. Nonetheless, external business and regulatory factors influence the trajectory of AI-discovered drugs, highlighting the biotech industry's complex innovation landscape.

The analysis emphasizes AI's transformative potential in drug discovery, implying that AI-discovered molecules could significantly improve clinical trial success rates. If current Phase I and II success rates are maintained and combined with historical Phase III success rates, the likelihood of a molecule passing through all clinical stages could nearly double, from 5-10% to 9-18%. This advancement may lead to increased pharmaceutical R&D productivity, allowing more drugs to be developed with fewer resources.

Looking ahead, advances in AI techniques such as OMICs data analysis, reverse translation, and large language models have the potential to improve clinical trial success rates, particularly in Phases II and III. Finally, AI promises to bring innovative medicines to patients faster and at a lower cost, with early success visible in preclinical and clinical workflows. The future of AI-powered R&D is set to reshape the landscape of drug development, providing exciting opportunities to improve efficiency and outcomes in the pharmaceutical industry17.

Table 5: Overview of AI Applications Across Drug Discovery and Development

Target Identification	• Machine learning models analyze genomic, proteomic, and transcriptomic datasets to identify novel disease-associated targets. • Network-based AI algorithms uncover molecular pathways, gene–gene interactions, and potential biomarkers. • Deep learning enables precise prediction of target–disease relationships using multi-omic integration.
Virtual Screening	• AI-driven high-throughput virtual screening accelerates identification of hit compounds from large chemical libraries. • Deep learning–based docking and scoring functions improve prediction of ligand–receptor binding affinity. • Generative AI models design new chemical structures with optimized biological activity and physicochemical properties.
ADMET Prediction	• Predictive models assess absorption, distribution, metabolism, excretion, and toxicity early in development, reducing costly failures. • AI supports physiologically based pharmacokinetic (PBPK) modeling for accurate dose estimation and metabolic profiling. • Toxicity prediction platforms evaluate hepatotoxicity, cardiotoxicity (e.g., hERG inhibition), mutagenicity, and off-target effects.
Clinical Trials	• AI improves patient recruitment by identifying eligible participants from electronic health records, genetic data, and real-world datasets. • Predictive analytics support adaptive trial designs, dose optimization, and endpoint forecasting. • Natural language processing (NLP) and monitoring tools track patient adherence, adverse events, and real-time study performance.
Post-Marketing Surveillance (PMS)	• Machine learning models analyze adverse event databases (e.g., FAERS, VigiBase) to detect early safety signals. • NLP extracts safety information from unstructured sources such as physician notes, patient reviews, and social media. • AI-powered pharmacovigilance systems provide continuous risk assessment, improve causality analysis, and support regulatory decision-making.

AI in the Regulatory Framework

USA: No AI-specific law; FDA regulates AI through existing medical device pathways. Key initiatives include the 2019 AI/ML SaMD Framework and the 2021 Action Plan focusing on lifecycle oversight, transparency, GMLPs, and bias reduction.

UK: MHRA's Change Programme, along with NICE/NHS frameworks, guides AI-based medical devices with emphasis on cybersecurity, clinical performance, and stakeholder engagement.

EU: The proposed AI Act introduces a risk-based approach; high-risk healthcare AI requires strict compliance, while low-risk tools follow voluntary codes of conduct.

Australia: TGA applies a risk-based model; 2021 reforms exclude low-risk consumer software and prioritise regulation of high-risk AI impacting patient safety.

China: NMPA enforces strict AI-MD regulations covering algorithm validation, device classification, software quality, cybersecurity, and total product lifecycle control.

Brazil: 2021 AI framework and 2022 draft law classify healthcare AI as high-risk, requiring risk assessments, transparency, and accountability from developers and providers.

Singapore: National AI Strategy supports safe innovation; HSA's SaMD guidelines and the "AI Verify" framework ensure ethical, transparent, and trustworthy AI use in healthcare.

AI in Post-Marketing Surveillance

Understanding Post-Market Surveillance (PMS)

A methodical procedure for keeping an eye on medical devices after they are put on the market is called post-market surveillance. It entails collecting information on how well the product is performing, responding to complaints, and resolving any unfavorable incidents. Maintaining patient safety and adhering to international regulations depend on effective PMS25.

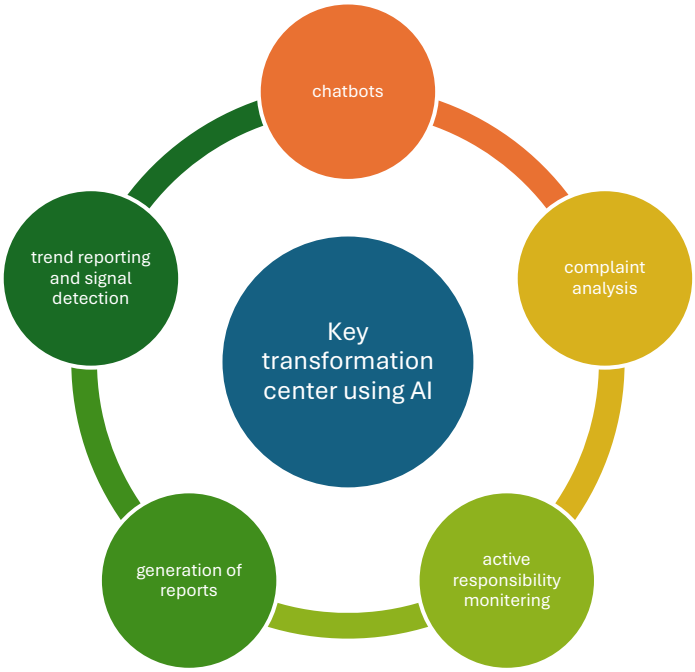

Figure 6: key transformation step using AI

- Post-marketing surveillance (PMS) is the systematic monitoring of a drug's safety and performance after it reaches the market. It uses tools such as adverse event reporting systems, electronic health records (EHRs), spontaneous reporting databases, social media monitoring, and real-world evidence platforms to identify safety issues that may not appear during clinical trials.
- AI enhances PMS by automating the analysis of these large and diverse datasets, enabling early detection of adverse events and safety signals. Machine learning models can identify hidden patterns, predict potential risks, and classify reports with greater accuracy. Natural language processing (NLP) extracts meaningful information from unstructured sources such as patient narratives, medical notes, and online reviews. AI-enabled dashboards and automated signal-detection systems provide real-time monitoring, improving responsiveness and regulatory decision-making.
- By accelerating data analysis, improving sensitivity to emerging risks, and reducing manual workload, AI strengthens pharmacovigilance and supports timely interventions to protect patient safety.31

Applications of Artificial Intelligence in the Pharmaceutical Industry

Area / Stage	Application of AI	Technologies / Methods Used	Major Functions / Benefits	Examples / Key Points
AI in Preclinical Trials	AI is used to identify promising drug candidates before laboratory and animal testing.	Machine Learning (ML), Deep Learning	Analyzes large biological and chemical datasets; predicts toxicity, metabolism, bioavailability, and possible side effects; eliminates unsuitable compounds at an early stage; saves time and resources.	AI also predicts drug–target interactions and identifies disease biomarkers. Deep learning analyzes images from cell cultures, tissues, and animal studies, reducing manual errors.
Investigational New Drug – Formulation Development	AI helps optimize pharmaceutical formulations and	QSPR, Expert Systems (ES), Artificial Neural Networks (ANNs),	Predicts drug stability, dissolution rate, porosity, and other physicochemical	AI-based systems can continuously monitor formulation

	physicochemical properties.	Decision-Support Systems	properties. Recommends suitable types and quantities of excipients. Formulation parameters can be adjusted using feedback mechanisms.	performance and optimize formulation variables.
Investigational New Drug – Piroxicam Formulation	Hybrid AI systems can optimize drug formulations.	Expert System + Artificial Neural Network (ANN)	The Expert System provides formulation recommendations using predefined knowledge, while the ANN learns relationships between formulation variables and dissolution profiles through backpropagation.	Guo and colleagues' hybrid system for piroxicam hard gelatin capsules demonstrated efficient and accurate formulation optimization.
AI + Mathematical Modeling	AI is integrated with computational models to understand pharmaceutical processes.	Computational Fluid Dynamics (CFD), Discrete Element Modeling (DEM), Finite Element Method (FEM), AI/ML	Studies powder flow, die filling, tablet compression, tablet geometry, and drug dissolution. Reduces experimental workload and improves prediction accuracy.	Integration of AI with CFD, DEM, and FEM accelerates development of high-quality dosage forms.
Investigational New Drug – Pharmaceutical Manufacturing	AI supports automated and optimized pharmaceutical manufacturing processes.	CFD, RANS, DNS, LES	Analyzes fluid flow, mixing efficiency, agitation, and stress distribution in manufacturing equipment such as stirred tanks.	CFD helps optimize manufacturing operations and equipment design. DNS and LES provide more detailed understanding of complex flow dynamics.
Automated Pharmaceutical Synthesis	AI enables automated synthesis and manufacturing of pharmaceutical compounds.	Chemputer, Chemical Assembly scripting, AI-driven automation	Automates chemical synthesis, improves reproducibility, reduces human intervention, and can achieve yields and purity comparable to conventional synthesis.	Chemputer has been used to synthesize drugs including sildenafil, diphenhydramine hydrochloride, and rufinamide.
AI in Granulation	AI predicts and optimizes the granulation endpoint during tablet manufacturing.	Machine Learning, Neuro-Fuzzy Logic	Establishes relationships between critical process variables and product responses. Predicts the optimal amount of granulation fluid, impeller speed, and impeller diameter.	Neuro-fuzzy systems have been applied to granulators with capacities ranging from 25 to 600 L, including geometrically similar and dissimilar granulators.
Discrete Element Method (DEM)	AI-supported DEM simulates the movement and interaction of individual powder particles.	DEM, AI/ML	Studies powder segregation, mixer design, mixer speed, tablet movement during coating, and tablet residence time in spray zones.	Improves process understanding, equipment optimization, and coating uniformity.

Tablet Manufacturing Optimization	AI optimizes machine operating parameters and reduces manufacturing defects.	ANN, Fuzzy Logic	Identifies relationships between machine parameters and defects such as tablet capping. Helps determine optimal machine settings.	Reduces production defects, manufacturing losses, and improves tablet quality.
Quality Control & Quality Assurance	AI automates tablet inspection and quality assessment.	Meta-Classifier, Tablet-Classifier, Machine Learning, ANN	Detects tablet defects and deviations from predefined quality standards. Provides rapid and real-time quality assessment.	Reduces manual inspection and improves consistency of pharmaceutical products.
Personalized Medicine	AI enables patient-specific dosage and formulation design.	AI-based decision-support systems, Machine Learning	Analyzes patient-specific clinical information to determine appropriate drug combinations and dosage regimens.	AI can also support the design of customized transdermal patches according to individual patient requirements.
AI in Quality Control & Quality Assurance	AI improves pharmaceutical product quality and process consistency.	Decision Trees, ANN, Real-Time Monitoring, QbD	Predicts product quality, optimizes manufacturing parameters, identifies deviations early, and reduces human error.	FDA's Quality by Design (QbD) approach focuses on controlling critical manufacturing parameters. AI supports data-driven QbD implementation.
Dissolution Prediction	AI predicts drug dissolution profiles to maintain batch-to-batch consistency.	Artificial Neural Networks (ANNs)	Uses manufacturing and formulation data to predict dissolution behavior accurately.	Helps ensure consistent quality between different production batches.
Lyophilization / Freeze-Drying	AI predicts important freeze-drying parameters and product characteristics.	ANN	Predicts product temperature and dried-cake thickness during lyophilization.	Helps maintain product quality and optimize freeze-drying conditions.
AI in Clinical Trials	AI improves patient recruitment, monitoring, adherence, and trial efficiency.	AI, Machine Learning, Predictive Analytics, Mobile Applications	Identifies suitable patients using genetic and clinical data; predicts promising candidates; monitors treatment adherence; reduces patient dropout; improves trial success and efficiency.	Clinical trials may take 6–7 years. AI can help address challenges such as poor patient selection, infrastructure limitations, and patient dropout.
Patient Recruitment in Clinical Trials	AI identifies patients who are most likely to meet trial eligibility criteria.	ML, Genetic Data Analysis, Clinical Data Analysis	Matches patients with appropriate clinical trials using genetic, medical, and clinical information.	Improves recruitment efficiency and increases the likelihood of successful trials.
Patient Adherence in Clinical Trials	AI-powered systems monitor whether patients follow treatment protocols.	AI Mobile Applications, Computer Vision, Digital Monitoring	Reminds patients to take medication, monitors adherence, and reduces dropout.	AiCure developed an AI-based mobile application reported to increase medication adherence by 25%

				in a Phase II schizophrenia clinical trial.
AI in Product Marketing	AI improves pharmaceutical marketing and product visibility.	SEO, Statistical Analysis, Particle Swarm Optimization (PSO), Neural Networks	Analyzes consumer behavior, market trends, and purchasing patterns. Supports targeted marketing, product positioning, resource allocation, and business growth.	Digital technologies and e-commerce platforms allow pharmaceutical companies to reach wider audiences.
AI in Market Prediction & Analysis	AI predicts customer demand, sales, and market performance.	Machine Learning, NLP, Statistical Analysis, Neural Networks, Time-Series Forecasting	Analyzes customer behavior, purchasing trends, search keywords, and market data. Forecasts product demand and sales.	Helps companies optimize marketing strategies, maintain inventory, reduce excess stock, and prevent medicine shortages.
AI in Digital Pharmaceutical Services	AI improves online access to medicines and healthcare services.	AI, NLP, Recommendation Systems, Digital Platforms	Allows customers to search for medicines, compare products, place orders, and track deliveries.	Online pharmacy platforms such as 1mg, Medline, Netmeds, and Ask Apollo use digital technologies to improve accessibility and customer service.
AI in Sales Prediction	AI predicts future pharmaceutical product demand.	Business Intelligence, Time-Series Forecasting, Real-Time Data Analysis	Predicts sales and demand, allowing companies to maintain optimal inventory levels.	Business Intelligent Smart Sales Prediction Analysis combines time-series forecasting and real-time data to support demand prediction.
AI in Drug Approval	AI supports pharmaceutical companies and regulatory agencies throughout the drug approval process.	Machine Learning, NLP, Predictive Analytics, Data Mining	Processes large datasets from preclinical studies, clinical trials, manufacturing, and post-marketing surveillance. Identifies patterns, predicts outcomes, and detects safety risks.	Supports evaluation of a drug's safety, efficacy, quality, and benefit–risk profile.
AI in Regulatory Submission	AI assists in preparing and reviewing regulatory documents.	Natural Language Processing (NLP), Machine Learning	Extracts relevant information, reviews scientific literature, checks data consistency, and reduces documentation errors.	Can make regulatory submissions more organized and efficient.
AI for Approval Prediction	AI estimates the likelihood of regulatory approval.	Predictive Modeling, Machine Learning	Compares new drug candidates with previously approved medicines and identifies factors associated with approval.	Can help pharmaceutical companies identify potential regulatory challenges earlier.
AI for Regulatory Review	AI can assist regulatory agencies in reviewing drug applications.	AI, NLP, Data Analytics	Helps identify missing or inconsistent information and prioritize applications for review.	Supports faster and more evidence-based regulatory decision-making.

AI in Pharmacovigilance	AI monitors the safety of medicines after approval.	Machine Learning, NLP, Real-World Data Analytics	Analyzes electronic health records, adverse-event reports, and real-world patient data to detect potential safety signals.	Helps identify rare or unexpected adverse effects earlier and strengthens post-marketing drug safety monitoring.
Overall Role of AI in Pharmaceuticals	AI integrates data analysis, prediction, automation, and intelligent decision-making throughout the pharmaceutical lifecycle.	AI, ML, Deep Learning, ANN, NLP, CFD, DEM, FEM, Expert Systems, Fuzzy Logic	Improves efficiency, reduces costs and experimental workload, enhances product quality, supports automation, improves patient selection and monitoring, and enables personalized pharmaceutical production.	AI contributes from drug discovery and preclinical development → formulation → manufacturing → quality control → clinical trials → marketing → regulatory approval → pharmacovigilance.

Summary of AI Applications Across the Pharmaceutical Lifecycle

Pharmaceutical Stage	Major AI Applications	Main Outcome
Drug Discovery & Preclinical Development	Drug candidate screening, toxicity prediction, drug–target interaction, biomarker identification, image analysis	Faster identification of promising and safer candidates
Formulation Development	QSPR, Expert Systems, ANN, formulation optimization	Improved formulation quality and dissolution
Process Development	CFD, DEM, FEM, AI-based modeling	Better understanding and optimization of pharmaceutical processes
Manufacturing	Chemputer, AI-controlled granulation, powder-flow modeling, tablet optimization	Automation, reproducibility, reduced waste, and improved efficiency
Quality Control & Assurance	Tablet classification, defect detection, ANN, decision trees, real-time monitoring	Consistent product quality and early detection of deviations
Personalized Medicine	Individualized dosage design, drug combinations, customized transdermal patches	Patient-specific treatment and dosage
Clinical Trials	Patient recruitment, adherence monitoring, predictive analysis	Faster recruitment, reduced dropout, improved trial efficiency
Marketing	SEO, consumer analysis, targeted marketing, demand prediction	Better product visibility and marketing performance
Market Analysis	Sales forecasting, NLP, time-series analysis, customer behavior analysis	Better demand forecasting and inventory management
Drug Approval	Regulatory document analysis, predictive models, data checking	More efficient regulatory review and decision-making
Post-Marketing / Pharmacovigilance	Adverse-event analysis, EHR analysis, real-world data analysis	Earlier detection of safety signals and improved drug safety

Key Advantages of AI in the Pharmaceutical Industry

Advantage	Impact
Time reduction	Accelerates drug discovery, formulation, manufacturing, clinical trials, and regulatory processes
Cost reduction	Reduces unnecessary experiments, material wastage, manual labor, and failed development programs
Improved accuracy	Provides accurate predictions and reduces human error
Process optimization	Identifies optimal manufacturing and formulation parameters
Automation	Reduces manual intervention in synthesis, inspection, and monitoring
Quality improvement	Enables continuous and real-time quality monitoring
Better patient selection	Improves clinical-trial recruitment and personalized treatment
Predictive capability	Predicts toxicity, dissolution, product quality, demand, and safety risks
Personalization	Supports patient-specific dosage forms and treatment regimens
Enhanced safety	Enables earlier identification of potential drug-related safety issues

Data-driven decision making	Converts large and complex datasets into actionable information
Regulatory support	Helps organize, analyze, and validate information required for drug approval

Challenges

AI adoption in drug discovery faces several significant challenges. A major concern is the availability and quality of training data, as incomplete, biased, or non-standardized datasets can lead to inaccurate predictions and limit model reliability. Ethical issues also arise, particularly regarding patient data privacy, consent, and the risk of algorithmic bias influencing research outcomes. Limited model transparency further complicates adoption, as many AI systems function as "black boxes," making it difficult to interpret how decisions are made. Robust validation and reproducibility remain important hurdles, since AI models often perform inconsistently across different datasets or laboratory settings. Additionally, regulatory gaps persist, with agencies still developing clear guidelines for evaluating AI-based tools in drug development. Finally, the need for advanced computational resources and specialized instruments can restrict widespread implementation, especially in resource-limited environments.32

Conclusion

Artificial intelligence is reshaping modern drug discovery by introducing advanced data-driven techniques that strengthen decision-making across the entire development pipeline. Its ability to analyze complex biological datasets, predict molecular behavior, and identify promising compounds enables faster and more informed target selection while reducing early-stage failures. AI-driven models are also improving preclinical and clinical evaluations through enhanced toxicity prediction, optimized trial design, and more precise patient stratification, supporting the development of safer and more personalized therapies. In the post-marketing phase, AI contributes to more effective pharmacovigilance by detecting emerging safety signals earlier than traditional methods. As algorithms continue to advance and access to high-quality biomedical data expands, AI is expected to play an even greater role in areas such as drug repurposing, multi-target drug design, and long-term outcome prediction. Moving forward, close collaboration between researchers, industry, and regulatory authorities will be essential to ensure ethical, transparent, and reliable implementation. Overall, AI holds significant potential to accelerate innovation and improve the safety and effectiveness of future therapeutics.

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