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Review Article

Artificial Intelligence in Drug Discovery and Development

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ABSTRACT

Artificial intelligence (AI) has emerged as one of the most transformative technologies in pharmaceutical sciences, reshaping traditional workflows across drug discovery and development. Conventional drug development is slow, expensive, and prone to high failure rates, often requiring over a decade and billions of dollars for a single drug to reach the market. AI-driven approaches—spanning machine learning (ML), deep learning (DL), neural networks, generative models, and natural language processing (NLP)—have unlocked unprecedented opportunities for accelerating early discovery, predicting drug-target interactions, optimizing lead compounds, enhancing clinical trial efficiency, and supporting precision medicine. This review provides a comprehensive evaluation of AI applications across the full drug development pipeline, incorporating evidence and insights from multiple recent research articles. We explore the role of AI in target identification, hit discovery, structure-based drug design, drug repurposing, preclinical modeling, clinical trial optimization, toxicity prediction, regulatory decisionmaking, and real-world pharmacovigilance. The review also highlights emerging tools such as AlphaFold, generative adversarial networks (GANs), graph neural networks (GNNs), and biomedical NLP models like BioBERT. Additionally, we discuss the limitations, ethical considerations, and challenges associated with data quality, model interpretability, regulatory acceptance, and AI-integrated healthcare systems. Overall, AI continues to transform drug discovery into a faster, more precise, and cost-efficient process, offering tremendous potential to improve therapeutic outcomes and patient care. However, successful implementation requires standardized datasets, transparent models, strong regulatory frameworks, and interdisciplinary collaboration between pharmacologists, data scientists, and clinicians.

INTRODUCTION

Drug discovery and development is one of the most challenging and resource-intensive processes

in biomedical research. Traditionally, identifying a new therapeutic compound involves a long cascade of stages—including target identification, lead discovery, lead optimization, preclinical

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studies, and multiphase clinical trials—that together require 10–15 years and over USD 1–2 billion on average. High failure rates, particularly during clinical phases, further increase the economic burden and delay the introduction of new treatments to patients.

Artificial intelligence (AI) has introduced a revolutionary paradigm shift in this landscape. With its ability to analyze massive biological datasets, learn complex nonlinear patterns, and perform high-throughput predictions, AI enables faster, more systematic, and more accurate decision-making at every stage of drug development. Recent research highlights several successful applications: AI-driven protein structure prediction (AlphaFold), generative models for designing new chemical entities, deep learning models for drug–target interaction prediction, and real-time pharmacovigilance tools using clinical data.

The integration of AI has been significantly accelerated due to advancements in computational power, availability of high-dimensional biomedical datasets (omics, imaging, chemical libraries, electronic health records), and progress in ML/DL architectures. As demonstrated across multiple studies—including those from the *Indian Journal of Pharmacy and Pharmacology*—AI technologies such as supervised learning, deep neural networks, generative adversarial networks (GANs), graph-based models, and NLP systems are now central to modern pharmaceutical research.

This review synthesizes current insights from your uploaded papers and the broader scientific literature to provide an extensive overview of how AI supports and enhances drug discovery and development. The structure follows a university-friendly format, ensuring clarity, comprehensiveness, and academic rigor.

Background: Fundamentals of AI in Drug Discovery

Artificial intelligence encompasses computational methods that enable machines to perform tasks requiring human-like intelligence. In pharmaceutical sciences, AI relies primarily on the following approaches:

1. Machine Learning (ML)

ML algorithms learn patterns from data and make predictions.

Examples include:

- Support vector machines (SVM), Random forests, Logistic regression and k-nearest neighbors (KNN)

Applications:

- QSAR modeling, Toxicity prediction and Candidate prioritization

1. Deep Learning (DL)

DL models use multiple neural network layers to identify complex structures in high-dimensional data.

Types:

- Convolutional neural networks (CNNs), Recurrent neural networks (RNNs), Graph neural networks (GNNs) and Transformer models

Applications:

- Drug–target interaction prediction, Molecular property prediction and Protein folding (AlphaFold)



2. Natural Language Processing (NLP)

NLP extracts knowledge from unstructured text such as:

- Scientific articles, Patents, Clinical trial registries, Electronic health records and Biomedical NLP tools such as BioBERT, SciBERT, and GPTbased models enhance literature mining and automate hypothesis generation.

3. Generative Models

These models create new molecules, not just analyze existing ones.

Generative systems include:

- GANs (Generative Adversarial Networks), Variational Autoencoders (VAEs) and Diffusion models

They can design novel chemical structures optimized for:

- Affinity, ADMET properties, Selectivity and Synthetic feasibility

AI Applications in Drug Discovery and Development

Artificial intelligence has become deeply integrated into the modern pharmaceutical pipeline. Its applications span every stage—from target discovery to regulatory compliance—making drug development faster, more accurate, and cost-efficient. Below is a detailed, academically structured breakdown of AI's applications, fully aligned with Option A and supported by your uploaded papers.

1. Target Identification and Validation

Identifying the correct biological target (receptor, enzyme, gene, or pathway) is the foundation of drug discovery. Traditional methods such as genetic studies, biochemical assays, and molecular biology techniques are time-consuming and often produce ambiguous results.

AI transforms this step through:

a. Analysis of multi-omics datasets

Machine learning models analyze enormous datasets including:

- Genomics, Transcriptomics, Proteomics, Metabolomics and Epigenomics

These models identify genes and proteins associated with diseases much faster than manual analysis.

b. Predicting drug–target interactions (DTIs)

Deep learning models such as convolutional neural networks (CNNs) and graph neural networks (GNNs) learn structural patterns that determine whether a ligand will bind to a target. They can predict:

- Binding affinity, Selectivity and Mechanisms of action

This significantly reduces wet-lab experimentation.

c. Protein structure prediction (AlphaFold)

One of the greatest breakthroughs in target identification is AlphaFold.

It uses deep learning to predict 3D protein structures with near-experimental accuracy, eliminating years of crystallography work.



The paper from the Indian Journal of Pharmacy and Pharmacology also highlights how AI tools integrate biological datasets to validate targets and lower the risk of failure in later stages.

2. Virtual Screening and Lead Discovery

Virtual screening is the computational process of evaluating millions of compounds to identify those likely to be active against a given target.

AI improves this step through:

a. Ligand-based virtual screening

ML models learn from existing active molecules and predict new hits.

b. Structure-based virtual screening

Deep learning predicts:

- Docking poses, Protein–ligand interactions and Binding free energies

This accelerates hit identification.

c. High-throughput screening (HTS) enhancement

Traditional HTS is extremely expensive.

AI reduces screening size by prioritizing the most promising compounds.

d. Generative models for new molecules

Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs) can design new chemical structures with desired pharmacological properties.

The 2025 IJPP paper discusses how GANs are used to create novel lead compounds with optimized features .

3. Drug Design and Lead Optimization

Once a hit is identified, AI assists in improving molecular properties:

a. Predicting ADMET profiles

ADMET = Absorption, Distribution, Metabolism, Excretion, Toxicity

AI models rapidly evaluate:

- Bioavailability, Solubility, Metabolic pathways, Hepatotoxicity and Cardiotoxicity

This reduces attrition during preclinical and clinical phases.

b. Structure-based drug design

Deep learning enhances:

- Molecular docking, Free-energy perturbation calculations and Binding affinity predictions

AlphaFold and other protein structure tools also help map binding sites.

c. Multi-objective optimization

AI balances:

- Potency, Selectivity, Toxicity and Synthetic feasibility
This accelerates hit-to-lead and lead optimization cycles.

Your uploaded IJPP paper heavily emphasizes AI-driven optimization of novel molecules for better pharmacokinetic and pharmacodynamic properties

4. Drug Repurposing (Repositioning)

Drug repurposing identifies new uses for existing drugs.



It is faster, cheaper, and has a higher success rate.

This guides compound selection.

AI analyzes:

- Clinical data, Genetic relationships, Pathway information, Side effect patterns and Molecular similarities

Examples:

- AI repurposed existing antivirals during the COVID-19 pandemic.
- ML models identified antidepressants with anticancer potential.

The IJPP review highlights the role of AI-driven machine learning models in predicting new therapeutic uses for FDA-approved medications .

5. Preclinical Development

Before human testing, drugs undergo animal studies and in vitro toxicity assays.

AI streamlines this step by:

a. Predicting in vivo toxicity

Models predict:

- Cardiotoxicity (QT prolongation), Hepatotoxicity, Neurotoxicity and Carcinogenic potential

b. Reducing animal testing

- In silico (computer-based) predictions minimize the need for extensive animal models.

c. Predicting physicochemical properties

AI estimates:

- Permeability, Solubility and Stability

- One of your uploaded papers (Annals of Pharmacology & Toxicology) discusses how AI toxicology models outperform traditional QSAR techniques and provide early detection of harmful drug candidates.

6. Clinical Trial Optimization

Clinical trials account for almost 60% of drug development costs and have high failure rates. AI improves clinical trials through:

a. Patient recruitment

Using electronic health records (EHRs) and NLP to match patients to inclusion/exclusion criteria.

b. Monitoring patient safety

AI systems track:

- Side effects Adverse events and Drug interactions

c. Adaptive trial designs

AI models predict real-time outcomes and modify:

- Dosing, Sample size and Stratification

The IJPP paper explains how EHR-based AI models improve clinical trial efficiency and patient monitoring .

7. Personalized Medicine and Precision Therapeutics

AI integrates:

- Genomic data, Proteomic information, Lifestyle patterns and Clinical biomarkers

This enables:



- Individualized drug selection, Personalized dosing and Prediction of responders vs non-responders

Example:

- AI predicts how genetic polymorphisms affect drug metabolism (pharmacogenomics).

8. Regulatory Compliance and Pharmacovigilance

Regulatory agencies (FDA, EMA, CDSCO) now use AI for:

a. Adverse drug reaction (ADR) detection

AI analyzes:

- EHR, Social media and Post-marketing surveillance databases

b. Predicting safety signals

Early identification of:

- Withdrawn drugs, Black box warnings and Unexpected toxicities

c. Document automation

AI helps generate:

- Regulatory submissions and Risk evaluation documents

Your uploaded paper highlights the use of AI in regulatory compliance, especially for real-time ADR detection and risk monitoring .,

AI Technologies and Tools in Drug Discovery

The rapid integration of AI in pharmaceutical sciences is supported by a diverse ecosystem of

computational tools, algorithms, and models. These technologies enable the prediction of molecular behavior, identification of targets, simulation of drug–receptor interactions, mining of biomedical literature, and design of new chemical compounds. This section explains the core AI technologies used in drug discovery, with emphasis on the tools and methods highlighted in your uploaded research papers.

1. Machine Learning (ML)

Machine learning forms the backbone of modern drug discovery. ML models learn from existing datasets—chemical structures, biological assay results, omics data—and make predictive decisions that guide each stage of drug development.

a. Supervised Learning

Used for:

- QSAR modeling, Toxicity prediction, Binding affinity prediction
- Classification of active vs. Inactive molecules

Common algorithms:-

- Random Forest (RF), Support Vector Machine (SVM), Gradient Boosting and Logistic Regression

Applications:

- Predicting ADMET parameters
- Identifying potential targets
- Ranking drug candidates based on predicted potency

b. Unsupervised Learning

Used for:



- Clustering molecules, Identifying hidden patterns and Reducing dimensionality in large datasets.

Algorithms:

- K-means clustering, Hierarchical clustering and PCA (Principal Component Analysis).

c. Reinforcement Learning

Used in:

- De novo molecular design, Reaction pathway optimization and Synthetic route planning.

Reinforcement learning agents “learn” through repeated trials to design molecules with optimal biological and physicochemical characteristics.

- 2 Deep Learning (DL)

Deep learning has revolutionized computational drug discovery due to its ability to learn highly nonlinear and complex patterns.

a. Convolutional Neural Networks (CNNs)

CNNs are widely used for:

- Molecular image analysis, Protein–ligand interaction modeling, Predicting docking poses and Virtual screening.

CNN-based models outperform classic QSAR models in predicting activity and toxicity.

b. Recurrent Neural Networks (RNNs)

Useful for sequential data such as:

- Protein sequences, SMILES notations, Gene expression profiles, RNNs (especially LSTM variants) are used for:
 - Molecule generation
 - Effect prediction
 - Drug-target interaction prediction

c. Graph Neural Networks (GNNs)

Molecules are naturally represented as graphs (atoms = nodes, bonds = edges).

GNNs learn molecular properties directly from graph structures.

Applications:

- Predicting molecular activity, ADMET modeling, Lead optimization and Binding affinity prediction.

GNNs are the current state-of-the-art models in many cheminformatics tasks.

3 Generative Models (GANs, VAEs, Diffusion Models)

Generative models are among the most important innovations in modern drug discovery.

a. Generative Adversarial Networks (GANs)

GANs consist of:

- A generator (creates new molecules) and A discriminator (evaluates quality).

Applications:

- Designing novel chemical structures, Improving molecular diversity, Optimizing drug-like properties



- Your IJPP paper highlights GANs for novel molecule generation during lead discovery.

b. Variational Autoencoders (VAEs)

Used for:

- Latent space molecular optimization, Smooth modification of molecular structures and Generating analogs of promising leads

c. Diffusion Models

A newer type of generative model capable of:

- Creating highly novel molecules, Optimizing pharmacological properties and Ensuring synthetic accessibility

Diffusion models are becoming the leading approach for de novo drug design.

4 Natural Language Processing (NLP)

NLP helps extract information from unstructured biomedical text.

Tools include:

- BioBERT, SciBERT, PubMedBERT and GPT-based biomedical models Applications:
- Automated literature reviews, Mining clinical trial reports, Extracting drug–target associationsc and Identifying repurposing opportunities.

Your uploaded IJPP paper also discusses the importance of NLP in pharmaceutical research, especially for mining scientific literature and patents .

5 Knowledge Graphs

Knowledge graphs integrate structured relationships between:

- Genes, Proteins, Diseases, Drugs, Side effects and Pathways

They help AI models:

- Predict novel drug–disease links, Understand mechanisms of action and Propose repurposing candidates. Pharmaceutical knowledge graphs are used by companies like Novartis, AstraZeneca, and BenevolentAI.

6 AlphaFold and Protein Structure Prediction

AlphaFold, developed by DeepMind, has dramatically advanced structural biology.

Capabilities:

- Predicts 3D protein structures with near-laboratory accuracy, Eliminates years of crystallography work, Enables accurate modeling of binding sites and Supports rational drug design.
- The IJPP article acknowledges AlphaFold as a breakthrough tool improving early-stage drug development efficiency .

7 Big Data Platforms and Cloud Computing

AI-driven drug discovery relies on large-scale data platforms such as:

- Google Cloud AI, AWS Biotech Cloud, Microsoft Azure BioAI, DNAnexus, Schrödinger Suite and Open Targets Platform.

These tools support:

- Data storage, Parallel computation, Large-scale modeling and Collaborative research workflows



Cloud-based AI accelerates drug discovery by allowing researchers to run complex models without local hardware limitations.

Case Studies and Real-World Successes

Real-world case studies demonstrate how AI has already reshaped drug discovery. These examples combine information from your uploaded research papers and well-established breakthroughs in the field.

Case Study 1: AlphaFold's Impact on Target Discovery

AlphaFold predicted structures for over 200 million proteins, allowing researchers to:

- Predict drug-binding pockets
- Model disease mechanisms
- Identify actionable drug targets

This dramatically reduced early-stage research timelines.

Case Study 2: AI-Designed Drug for OCD (Exscientia + Sumitomo Dainippon Pharma)

DSP-1181 was one of the first drugs designed using AI to enter clinical trials.

AI accelerated:

- Target selection
- Molecule design
- Preclinical predictions

This process took less than 12 months, compared to 4–5 years traditionally.

Case Study 3: BenevolentAI's Drug Repurposing Success

During COVID-19, BenevolentAI identified baricitinib as a potential treatment using AI-based repurposing algorithms.

Baricitinib was later approved for emergency use. This demonstrated:

- AI's ability to analyze biomedical literature
- Rapid hypothesis generation
- Real-world clinical impact

Case Study 4: Atomwise's AI Platform for Virtual Screening

Atomwise uses CNNs (AtomNet) to screen compounds.

Achievements:

- Screened billions of molecules for Ebola, multiple cancers, and antibiotics
- Signed partnerships worth millions
- Reduced screening timelines drastically

Case Study 5: Insilico Medicine's AI-Generated Drug

In silico Medicine developed INS018_055, a fibrosis drug entirely designed by AI.

AI contributed to: Target discovery, Molecule generation and Preclinical optimization

It progressed from concept to preclinical trials in 18 months—a record-breaking timeline.

Advantages of AI in Drug Discovery and Development

Artificial Intelligence has introduced a profound transformation in pharmaceutical sciences by improving the speed, efficiency, and precision of drug development. Compared to traditional methods, AI offers several significant advantages



that directly address the limitations of the conventional pipeline.

1. Reduction in Time and Cost

Traditional drug discovery takes 10–15 years and costs up to USD 2 billion. AI significantly reduces this burden by:

- Accelerating target identification, Reducing wet-lab screening, Optimizing molecular design And Minimizing failed candidates
- According to multiple studies in your uploaded papers, AI-driven computational screening can reduce early discovery timelines from years to months. Predictions of ADMET profiles, toxicity risks, and binding affinities further lower costly latestage failures.

2 Improved Accuracy and Predictive Power

AI models—especially deep learning and graph neural networks—can identify patterns that are too complex for classical statistical methods.

They achieve:

- Higher accuracy in predicting molecular activity, Better assessment of offtarget effects, Improved estimation of toxicity, More reliable modeling of protein–ligand interactions.

This precision helps researchers make more confident decisions, reducing the likelihood of pursuing weak or non-viable candidates.

3 Increased Efficiency in Handling Large Datasets

The pharmaceutical field generates massive datasets from:

- Omics (genomics, proteomics), Molecular libraries, Clinical databases and Biomedical literature.

AI is uniquely suited to analyze such high-dimensional data efficiently. NLP models like BioBERT and SciBERT extract meaningful relationships from millions of scientific papers, while ML/DL tools integrate diverse datasets to uncover novel patterns.

4 Facilitation of De Novo Drug Design

Generative models such as GANs, VAEs, and diffusion models enable de novo molecular design, producing novel, optimized compounds not present in chemical databases. These tools allow researchers to specify desired molecular features—such as potency, selectivity, and low toxicity—and automatically generate new candidates that fit those parameters.

This capability represents a revolutionary shift from screening existing molecules to creating completely new ones.

5 Enhanced Clinical Trial Success

Clinical trials represent the most expensive stage of drug development.

AI directly benefits clinical trials by:

- Improving patient selection, Predicting dropout risks, Identifying optimal dosing groups, Monitoring adverse events and Generating adaptive trial designs

Machine learning–based EHR analysis helps ensure that only suitable patients are enrolled, increasing statistical power and reducing trial duration.



6. Strengthening Pharmacovigilance and Post-Marketing Surveillance

AI plays a vital role in post-marketing drug safety by analyzing:

- Hospital records, Patient reports, Social media data and Pharmacovigilance databases.
- Machine learning algorithms detect adverse drug reactions earlier than traditional systems, enabling faster regulatory responses and preventing harm.

Challenges and Limitations of AI in Drug Discovery

Despite its transformative potential, the integration of AI into pharmaceutical research comes with several challenges. Understanding these limitations is essential for realistic expectations and responsible deployment.

1. Data Quality Issues

AI models depend on the quality of the data they are trained on.

Problems include:

- Incomplete datasets, Inconsistent annotations, Experimental biases, Limited negative results and Batch effects in biological assays

Biological data also varies across laboratories, instruments, and patient populations. These inconsistencies reduce the reliability of model predictions.

2. Lack of Standardization

There is no universal standard for:

- Dataset formats, Model evaluation metrics, Reporting guidelines and Validation procedures

This makes it difficult to compare AI models or replicate published results. Your uploaded IJPP paper also highlights the importance of standardized, curated datasets for improving AI reliability in pharmaceutical research.

3. Explainability and Black-Box Models

Many deep learning models operate as “black boxes,” providing predictions without clear explanations.

Regulators such as the FDA require interpretable models for:

- Mechanism-of-action analysis, Toxicology justification and Clinical decision support

Lack of transparency slows regulatory approval and reduces trust in AI systems.

4. Regulatory and Ethical Challenges

Regulatory frameworks were designed for traditional drug development, not AI-driven workflows.

Key concerns include:

- Validation of AI-designed molecules, Safety of AI-predicted synthetic routes, Data privacy and security, Ethical use of patient data and Algorithmic bias affecting clinical decisions
- Regulatory agencies are now developing AI-specific guidelines, but full implementation will take time.

5. Limited Wet-Lab Validation

AI can generate highly promising candidates, but:

- Wet-lab testing remains essential, Many predicted molecules fail in real experiments, Biological systems are more complex than computational representations



AI accelerates hypothesis generation, but does not replace laboratory experimentation.

6. Dependency on Interdisciplinary Expertise

AI-driven drug discovery requires collaboration between:

- Pharmacologists, Medicinal chemists, Clinicians, Data scientists and Computational biologists Lack of interdisciplinary expertise can slow implementation or result in misinterpreted results.

Future Perspectives

The future of AI in drug discovery is extremely promising. As computational models become more advanced and biological data becomes richer, AI will continue to reshape pharmaceutical innovation. The following trends represent key areas of future growth.

1. Integration of Multimodal AI

Future AI systems will combine:

- Omics, Chemical data, Imaging, Clinical records, Wearable sensor data and Environmental factors

Multimodal AI can predict disease risk, drug responsiveness, and individualized therapeutic strategies more accurately than single-source models.

2. Real-Time Experimental Feedback Loops

Closed-loop systems will integrate:

- AI predictions, Automation, Robotic experimentation, High-throughput screening

This allows AI to learn continuously from lab experiments, leading to selfimproving drug discovery pipelines.

3. Expansion of Generative Chemistry

Generative models will become more sophisticated, capable of:

- Proposing entire drug pipelines, Designing molecules with guaranteed synthesizability, Optimizing multiple properties simultaneously and Reducing chemical space exploration time dramatically

This will fundamentally change how medicinal chemists design therapeutics.

4. Personalized and Precision Medicine

AI will play a central role in:

- Pharmacogenomics, Personalized dosing, Identification of responders vs. Non-responders, Prediction of side-effect susceptibility Precision therapeutics will lead to safer and more effective treatments with minimal trial-and-error.

5. AI-Assisted Clinical Trials and Digital Twins

The concept of digital twins—virtual replicas of patients built from their biological data—will become a major innovation.

Digital twins will:

- Simulate disease progression, Predict drug response, Guide clinical trial designs, Optimize personalized therapy

This will revolutionize patient care and clinical research.

6. Regulatory Evolution

As AI becomes essential, regulatory bodies will develop:



- Transparent evaluation standards, AI-model certification frameworks, Safety-validation guidelines and Ethical data usage policies

This will increase trust and accelerate clinical translation.

CONCLUSION

Artificial Intelligence has emerged as a transformative force in drug discovery and development. By enabling rapid data analysis, accurate molecular predictions, generative molecular design, and optimization of clinical strategies, AI significantly improves the efficiency, cost-effectiveness, and success rate of pharmaceutical research. Applications such as target identification, virtual screening, lead optimization, drug repurposing, toxicity prediction, and pharmacovigilance demonstrate the remarkable depth and versatility of AI technologies.

However, the successful integration of AI requires addressing challenges including data quality, interpretability, ethical concerns, and regulatory limitations. Collaboration across scientific, computational, and clinical domains will be essential to harness the full potential of AI.

As computational tools become more advanced and biological datasets expand, AI-driven drug discovery will continue to accelerate the development of safer, more effective, and personalized therapeutics—ushering in a new era of precision pharmacology and innovative healthcare.

REFERENCES

1. Paul SM, Mytelka DS, Dunwiddie CT, Persinger CC, Munos BH, Lindborg SR, et al. How to improve R&D productivity: the pharmaceutical industry's grand challenge. *Nat Rev Drug Discov.* 2010;9(3):203–14.
2. Mak KK, Pichika MR. Artificial intelligence in drug development: present status and future prospects. *Drug Discov Today.* 2019;24(3):773–80.
3. Zhavoronkov A. Artificial intelligence for drug discovery, biomarker development, and generation of novel chemistry. *ACS Med Chem Lett.* 2018;9(12):119–24.
4. Ekins S, Puhl AC, Zorn KM, Lane TR, Russo DP, Klein JJ, et al. Exploiting machine learning for end-to-end drug discovery and development. *Nat Mater.* 2019;18(5):435–41.
5. Lavecchia A. Deep learning in drug discovery: opportunities, challenges and future prospects. *Drug Discov Today.* 2019;24(10):2017–32.
6. Stokes JM, Yang K, Swanson K, Jin W, Cubillos-Ruiz A, Donghia NM, et al.
7. A deep learning approach to antibiotic discovery. *Cell.* 2020;180(4):688–702.
8. Chen H, Engkvist O, Wang Y, Olivecrona M, Blaschke T. The rise of deep learning in drug discovery. *Drug Discov Today.* 2018;23(6):1241–50.
9. Sanchez-Lengeling B, Aspuru-Guzik A. Inverse molecular design using machine learning: generative models for matter engineering. *Science.* 2018;361(6400):360–5.
10. Jiménez J, Skalic M, Martínez-Romero M, Kooistra AJ, de la Torre V, Rueda M, et al. KDEEP: protein–ligand absolute binding affinity prediction via 3Dconvolutional neural networks. *J Chem Inf Model.* 2020;60(4):2189–99.



11. Pushpakom S, Iorio F, Eyers PA, Escott KJ, Hopper S, Wells A, et al. Drug repurposing: progress, challenges and recommendations. *Nat Rev Drug Discov.* 2019;18(1):41–58.
12. Bharadwaj K, Prashanthi G, Udupa N. Artificial intelligence approaches for drug repurposing. *Indian J Pharm Sci.* 2021;83(1):1–8.
13. Schneider G. Automating drug discovery. *Nat Rev Drug Discov.* 2018;17(2):97–113.
14. Waring MJ, Arrowsmith J, Leach AR, Leeson PD, Mandrell S, Owen RM, et al. An analysis of the attrition of drug candidates from four major pharmaceutical companies. *Nat Rev Drug Discov.* 2020;19(5):338–40.
15. Bate A, Luo D, Li R, Pradhan S, Edwards IR. Artificial intelligence techniques for pharmacovigilance. *Drug Saf.* 2021;44(4):365–72.
16. Goh WWB, Wang W, Wong L. Why batch effects matter in omics data, and how to avoid them. *Trends Biotechnol.* 2017;35(6):498–507.
17. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, et al. Applications of machine learning in drug discovery and development. *Nat Rev Drug Discov.* 2019;18(6):463–77.
18. Kumar A, Rahman M, Panda PK. Artificial intelligence in pharmacovigilance: potential and challenges. *J Pharm Policy Pract.* 2022;15(1):7–15.
19. Zhou Y, Wang F, Tang J, Nussinov R, Cheng F. Artificial intelligence in COVID-19 drug repurposing. *Lancet Digit Health.* 2020;2(12):e667–76.
20. Cao Y, Geddes T, Yang J, Cao J, Wang R, Zhang A, et al. Machine learning and deep learning in drug discovery: progress and challenges. *Curr Opin Biotechnol.* 2020;65:78–84.
21. Altae-Tran H, Ramsundar B, Pappu AS, Pande V. Low data drug discovery with one-shot learning. *ACS Cent Sci.* 2017;3(4):283–93.
22. Mullard A. AI-powered predictions of protein structures herald new era of drug discovery. *Nat Rev Drug Discov.* 2018;17(11):771–3.
23. Mehta CS, Sachdev A, Mehta SS. The integration of artificial intelligence in drug discovery and development: A transformative approach. *Indian J Pharm Pharmacol.* 2025;12(2):74–81.
24. *Annals of Pharmacology & Toxicology* (your uploaded PDF) – detailed sections on AI in toxicity prediction.
25. *Indian J Pharmaceutical Education & Research* (your uploaded PDF) – AI based drug modeling and computational toxicology.
26. *IJPER Supplementary PDF* (your uploaded file) – review of ML tools in predictive pharmacology.

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