



Review Article

Artificial Intelligence in Drug Discovery and Development

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Abstract:

Artificial Intelligence (AI) is rapidly transforming drug discovery and development by improving efficiency, accuracy, and speed. Traditional drug development is a lengthy and costly process that may take 10-15 years and require billions of dollars to bring a single drug to market. AI helps overcome these limitations by analysing large biological datasets, predicting outcomes, and supporting decision-making throughout different stages of drug development. Machine learning and generative AI models assist in target identification, de novo drug design, virtual screening, lead optimisation, and prediction of ADEMT properties, thereby reducing late-stage failures and improving overall success rates. AI also plays an important role in clinical trial optimisation through better patient selection, real-time monitoring, and outcome prediction. Growing investments and high adoption rates in the pharmaceutical industry highlight the expanding AI market and its economic impact. Despite its advantages, challenges such as data quality issues, high implementation costs, lack of interpretability, ethical concerns, and regulatory complexities remain significant. In India, AI-based drug discovery is guided by CDSCO regulations, ICMR ethical guidelines, NDCTR 2019, and the Digital Personal Data Protection Act, 2023 to ensure safety and compliance. Overall, AI has strong potential to revolutionize pharmaceutical research by accelerating innovation, reducing costs, and enabling personalized medicine.

Keywords: Artificial Intelligence (AI), Drug Discovery, Molecular Design, validation.

Introduction

AI is increasingly becoming an essential component of pharmaceutical industry, particularly in drug discovery and development. By enhancing efficiency, accuracy, and speed. It has evolved from a “high tech experiment” into the backbone of the pharmaceutical research.

Traditional drug development is a long, expensive and complex process that often take 10-15 years and cost billions of dollars to bring a single drug to market. AI helps to overcome

these challenges by analysing large data, predicting results, and supporting decisions. As a result, drug discovery timelines can be reduced from years to months, while also lowering costs and improving success rates.

Machine learning and generative AI models play a crucial role in this transformation. They assist in streamlines target identification, molecular design, virtual screening, and predictive toxicology.

The use of AI has gained significant attention in recent years as a potential means of revolutionising the pharmaceutical industry.

According to latest surveys, 80% of pharmaceutical and life-science professionals use AI for drug discovery.

Recent developments in AI show the potential for quick, affordable drug discovery and development.

A number of biotechnology, software and pharmaceutical firms are also working hard to incorporate AI into the research and development of new medicines. To improve the search for innovative oncology medicines, Pfizer joined with IBM Watson Health, an AI platform in 2016.

Furthermore, AI enhance accuracy and precision in drug design by identifying toxicity, solubility and stability. It also supports drug interactions, drug therapy monitoring and formulary selection, contributing to safer and more effective treatments.

Drug Discovery is a process which aims at identifying a compound therapeutically useful in curing and treating diseases. This process involves the identification of candidates, synthesis, characterization, validation, screening and assays for therapeutic efficacy.

Once a compound has shown its significance in these investigations, it will initiate the process of drug development earlier to clinical trials.

New drug development process must continue through several stages in order to make a medicine that is safe, effective, and has approves all regulatory requirements.

AI Market Growth

- AI technology in cancer diagnosis is projected to grow at a compound annual growth rate (CAGR) of about 90% from 2021 to 2028.
- The global AI market in genomics is expected to grow at an annual rate of approximately 52.7% between 2021 and 2028.

- Studies report that nearly 95% of pharmaceutical companies are investing in artificial intelligence capabilities.
- A study found that the use of AI could reduce drug development timelines to nearly four years and result in savings of about \$26 billion.
- The application of AI in clinical trials can reduce trial duration and overall costs by approximately 70-80%.

Role of AI in drug discovery and development

Artificial Intelligence plays a significant role in accelerating the drug discovery process by analysing vast biological data, designing novel compounds, optimising clinical trials, identifying and validating drug targets by studying disease pathways, gene expression. Machine learning and deep learning algorithms enable virtual screening of large compound libraries, allowing researchers to predict molecular effectiveness and select promising drug candidates efficiently.

It improves accuracy in predicting toxicity, solubility, stability, and pharmacokinetic parameters at early stages, thereby reducing failure rates in later phases. Additionally, AI supports personalised medicine by enabling the selection of suitable drug therapies based on patient-specific data.

AI also enhances the integration of multi-omics data such as genomics, proteomics, and metabolomics to better understand complex disease mechanisms. By identifying hidden patterns in large datasets, AI supports biomarker discovery and improves target validation.

Furthermore, AI-driven predictive models help in repurposing existing drugs for new therapeutic indications, significantly reducing development time and cost. Automation powered by AI improves laboratory workflows, data management, and real-time analysis, increasing overall research productivity.

AI tools also assist in risk assessment by forecasting potential adverse drug reactions before clinical testing. This proactive approach

improves patient safety and strengthens regulatory compliance. As computational power and data availability continue to grow, AI is expected to further streamline innovation and enhance collaboration between pharmaceutical industries and research institutions.

Key applications of AI in Pharma

Drug Discovery and development is the systemic, multi-year process of identifying, testing, and approving new medication to treat diseases, ensuring they are safe and effective. It involves target identification, hit-to-lead optimisation, and preclinical/ clinical trials, transforming potential molecules into market-ready therapeutic agents.

- **Target Identification & Validation:** AI analyses biological data to find novel disease targets. Scientist identify specific proteins, genes, or molecular pathways associated with a disease to develop treatments that interact with them.
- **De Novo Drug Design:** Generative AI creates novel molecular structures designed to bind specific targets.
- **Virtual Screening:** Rapidly filters compound libraries to identify the most promising candidates, as seen in partnerships like NVIDIA/ Recursion.
- **Predicting ADMET Properties:** AI models predict Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) early, reducing late-stage failures.
- **Drug Repurposing:** Identifying new therapeutic uses for existing approved drugs, which significantly lowers development costs.
- **Molecular Design and Optimisation:** Machine learning and generative AI help in designing new molecules and optimising their chemical structures.
- **Improved success rate:** Early prediction of failures increases overall success in drug development.
- **Clinical Trial Optimisation:** Testing in humans to confirm safety, determine optimal dosages and verify effectiveness in large patient populations. AI aids in patient selection, recruitment, and monitoring, cutting trial times by 15-30%.
- **Lead Optimisation & Toxicity Prediction:** AI predicts pharmacokinetic properties and potential toxicity, prioritising the most effective, safe candidates.
- **Hit Identification & High-Throughput Screening (HTS):** Researchers test thousands of compounds via computer simulations (virtual screening) or laboratory tests- to find molecules that interact with the disease target.
- **Advancement in Personalised Medicine:** Utilising genetic data to create targeted therapies that are more specific, effective, and tailored to individual patient profiles.
- **Regulatory Approval and Post-Market Surveillance:** Submitting data (e.g., NDA/MAA) for authorisation by agencies like the FDA, followed by continuous monitoring (Phase IV) for long-term safety.

The entire, long, and expensive process is crucial for creating, for example, new treatments for cancer, infectious diseases, and chronic conditions like Alzheimer's.

Challenges and Limitations of AI

1. Data Quality and Availability- AI models require large, high-quality datasets. Incomplete, biased, or inaccurate data can lead to unreliable predictions.
2. High Cost of Implementation- Developing and maintaining AI systems require expensive infrastructure, skilled professionals, and computational resources.
3. Lack of Interpretability (Black Box Problem)- Many AI models do not clearly explain how predictions are made, reducing trust among researchers and regulators.
4. Regulatory and Ethical Challenges- Regulatory approval of AI-driven drug

discovery tools is complex due to lack of clear guidelines.

5. Dependency on Existing Knowledge- AI largely relies on existing data and may fail to identify completely novel drug mechanisms.
6. Skilled workforce requirement- There is a shortage of professional trained in both AI and pharmaceutical sciences.
7. Data Privacy and Security Concerns- Use of patient data raises concerns regarding data privacy and cybersecurity.
8. Limited Generalisability- AI models trained on specific datasets may not perform well across different populations, diseases, or geographical regions due to variations in biological and clinical data.
9. Integration with Traditional Research Methods- Combining AI tools with conventional laboratory and clinical workflows can be technically complex and time-consuming.
10. Regulatory Uncertainty- Lack of standardised global guidelines for AI-based drug discovery tools may delay approvals and commercialisation.

Indian Regulations of AI

AI regulation in Indian drug discovery is rapidly evolving, moving from a fragmented, sector-specific approach toward a centralised framework to ensure safety and ethical AI use in pharmaceutical R&D. Key components include ICMR ethical guidelines, the Digital Personal Data Protection Act, 2023, and Medical Device Rules, 2017 (covering AI software), with the CDSCO (Central Drugs Standard Control Organisation) focusing on enhancing efficiency, transparency, and data integrity.

1. Central Drugs Standard Control Organisation (CDSCO)- It regulates drugs, clinical trials and new drug approval in India. AI-based drug discovery outputs must be supported by experimental and clinical evidence before approval.

2. Indian Council of Medical Research (ICMR) Guidelines- It provides ethical guidelines for biomedical research. AI tools using patient or clinical data must follow ethical principles, consent, and data protection norms.
3. New Drugs and Clinical Trials Rules (NDCTR), 2019- Governs clinical trials and new drug development.
4. NITI Aayog- Ethical AI Framework- Promotes responsible use of AI in healthcare and pharma.
5. ICMR- CDSCO Oversight in Clinical Trials- AI-assisted drug discovery must comply with GCP (Good Clinical Practice) guidelines. Final decision remains under human regulators and ethics committee.
6. Medical Device Regulations- AI software and tools intended for medical purposes are regulated under the Medical Device Rules, 2017 (amended 2020), which require validation of safety and efficacy.

Thus, India adopts an innovative- friendly and ethical approach to regulate AI in drug discovery through established pharmaceutical regulations, ethical standards, and data protection laws.

AI techniques Used in Drug Discovery

In 2026, the landscape of drug discovery has shifted from “AI-assisted” to “AI-first”. AI techniques in drug discovery accelerate R&D by analyzing complex biological data using machine learning (ML), deep learning (DL), and generative AI.

- **Machine Learning (ML) & Deep Learning (DL):** Algorithms are used for classifying data and predicting drug-target interactions, such as using neural networks (CNNs, RNNs) to predict binding affinity (e.g., DeepDTA, PADME). Example; DeepMind developed AlphaFold for accurate protein structure prediction.
- **Natural Language Processing (NLP):** Extracts scientific literature and patent

databases for information on drug targets and biological relationships.

- **Generative AI (De Novo Design):** Algorithms, such as generative adversarial networks (GANs) and variational auto-encoders (VAEs), create new molecular structures with desired properties from scratch.
- **Unsupervised Learning:** Techniques like K-means clustering and Principal Component Analysis (PCA) group compounds based on similarities.
- **Multi- Omics Data Integration:** AI integrates genomics, proteomics, and metabolomics data to identify disease pathways and personalise medicine.
- **Virtual Screening (VS):** AI enables large-scale, accelerated screening of chemical libraries to identify hits, reducing reliance on physical, high-throughput experiments.
- **Graph Neural Networks (GNNs):** Molecules are naturally represented as graphs (atoms as nodes, bonds as edges). GNNs are specifically designed to predict molecular properties and toxicity by “understanding” the 3D geometry and connectivity of a drug candidate better than standard neural networks.
- **Reinforcement Learning (RL):** Used in “Goal- Directed” molecule generation. AI “agents” are rewarded for designing molecules that meet specific criteria (like low toxicity and high solubility), allowing the system to learn the best chemical “moves” over time.
- **Digital Twins & Simulation:** AI creates virtual models of human biological systems. This allows researchers to simulate how a drug might react in a human body before it ever enters a clinical trial, significantly reducing the risk of unforeseen side effects.
- **Dimensionality Reduction (PCA/t-SNE):** Simplifies high- dimensional data, helping to visualise chemical space and identify patterns.

Future scope of AI

The future of AI in drug discovery is promising, with potential to transform drug development into a faster, cost- effective, and patient-centric process. AI is poised to revolutionise drug discovery by reducing development timelines by 1–2 years and cutting costs. Future applications focus on generative AI for designing novel molecules, accelerated target validation, and personalized medicine using Multi-omics data. With continuous advancements in computational power, data integration, and algorithm innovation, AI is expected to become an indispensable pillar of next generation drug discovery.

- **Synergistic Drug Combinations:** AI will identify optimal multi-drug combinations, improving efficacy and reducing side effects for complex diseases like cancer.
- **Faster Drug Development:** AI will significantly reduce the time required to identify and develop new drug candidates, shortening the traditional 10-15 year drug development timeline.
- **Streamlined Clinical Trials:** AI will optimise trial design by identifying suitable participants via EHR(electronic health records) analysis, predicting outcomes, and monitoring patients in real-time, potentially reducing trial lengths by 15-30%.
- **Discovery of Novel Drugs:** Advanced AI models will help discover new drug molecules and mechanisms not identified by traditional methods.
- **Integration of Multimodal Data:** Future AI systems will combine genomic, proteomic, metabolomics, transcriptomics and imaging data to create a comprehensive understanding of diseases for personalised treatment, discover novel biomarkers and enable system- level drug discovery.
- **Advanced Protein Structure and Target Prediction:** Following breakthroughs like AlphaFold developed by DeepMind, AI will

further improve structure-based drug design and target validation.

- Drug Repurposing and Rare Disease Treatment: AI will identify new therapeutic applications for existing drugs by analysing biological pathways and clinical data. This is especially promising for rare diseases, emerging infectious diseases and pandemic preparedness.
- Ethical AI and Regulatory Advancements: Future developments will also focus on transparent AI models, regulatory frameworks for AI-driven drug approvals, Data privacy and security. Regulatory bodies worldwide are expected to integrate AI guidelines into pharmaceutical evaluation processes.

Conclusion

This review showed that integrating AI can revolutionise drug discovery and development. Utilising machine learning algorithms, deep learning techniques, and data analytics, AI can expedite target identification, optimise lead compounds, and predict pharmacokinetics and toxicity. This aims to promote the application of AI in drug discovery, addressing current challenges, encourage collaborative efforts among stakeholders, ensure the protection of intellectual property, and outline a future blueprint in which AI plays a crucial role in advancing pharmaceutical research.

Using the latest AI- based technologies will not only speed up the time needed for the products to come to the market, but will also improve the quality of products and the overall safety of the production process, and provide better utilisation of available resources along with being cost- effective, thereby increasing the importance of automation. AI can not only Sid

quick and hassle-free hit compound identification, but also contribute to suggestions of synthesis routes of these molecules along with the prediction of the desired chemical structure and an understanding of drug-target interactions and its SAR.

The growing levels of interest and attention from researchers, pharmaceutical companies, and regulatory agencies, combined with the potential benefits of AI, make this an exciting and promising area of research, with the potential to transform the drug discovery process.

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