Research Article

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# Artificial intelligence and machine learning in drug discovery-a review

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**Abstract**

The emergence of artificial intelligence (AI) and machine learning (ML) has revolutionized various sectors, including healthcare and pharmaceutical industries. Among the most transformative applications is their role in drug discovery and development. Traditionally a costly, laborious, and time-consuming process, drug discovery has significantly benefited from the integration of AI and ML technologies, enabling rapid identification of potential drug candidates, target identification, drug repurposing, and prediction of pharmacokinetics and toxicity. This article explores the principles, applications, benefits, challenges, and future perspectives of AI and ML in drug discovery, supported by contemporary references.

***Key Words:*** AI, drug discovery, machine learning.



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## Introduction

Drug discovery is a complex, multi-stage process involving target identification, compound screening, lead optimization, preclinical studies, and clinical trials. On average, the development of a new drug takes 10–15 years and costs around $2.6 billion USD [1]. The high attrition rate of candidate drugs in clinical trials is a significant contributor to these costs. AI and ML offer a paradigm shift in drug discovery by enabling data-driven decision-making, pattern recognition, and predictive modeling to accelerate and improve this process.

AI refers to computer systems capable of performing tasks that typically require human intelligence, such as reasoning, learning, and decision-making. ML, a subset of AI, involves algorithms that learn from data to make predictions or decisions without being explicitly programmed [2]. In the context of drug discovery, these technologies analyze vast datasets from genomics, proteomics, cheminformatics, and clinical trials to identify drug candidates, predict efficacy, and foresee adverse reactions.

## Applications of AI and Ml in Drug Discovery

### Target Identification and Validation

Identifying and validating disease-related targets is the cornerstone of successful drug discovery. AI algorithms can process genomic, proteomic, and transcriptomic datasets to uncover novel targets associated with diseases. ML models, especially deep learning networks, have been used to analyze gene expression data to identify disease biomarkers and actionable targets [3].

Natural language processing (NLP), a branch of AI, is used to mine scientific literature and clinical trial data to extract relevant information about potential drug targets [4].

### Hit Identification and Virtual Screening

Once a target is identified, the next step is to find molecules (hits) that can bind to and modulate the target. Traditional high-throughput screening (HTS) is resource-intensive. AI can expedite this process through virtual screening techniques using deep learning and quantitative structure-activity relationship (QSAR) models [5].

Generative models such as Variational Autoencoders (VAEs), Generative Adversarial Networks (GANs), and Reinforcement Learning (RL) have shown promise in designing novel molecules with desirable properties [6].

### Lead Optimization

Lead compounds often need structural modifications to improve efficacy, selectivity, and pharmacokinetic properties. ML models can predict the effect of chemical modifications on biological activity, reducing the number of iterations required [7].

Bayesian optimization, random forests, and support vector machines (SVMs) are among the commonly used techniques for optimizing drug-like properties such as ADMET (Absorption, Distribution, Metabolism, Excretion, and Toxicity) [8].

### Drug Repurposing

Drug repurposing involves identifying new therapeutic uses for existing drugs, offering a faster and more cost-effective route to drug development. AI models can integrate multi-omics data and disease-drug interaction networks to find potential repurposing opportunities [9].

For instance, AI played a pivotal role during the COVID-19 pandemic in identifying repurposable drugs like remdesivir and baricitinib [10].

### Prediction of Admet Properties

Many drug candidates fail due to poor pharmacokinetics or toxicity. Predicting these properties early can reduce late-stage failures. ML models trained on experimental ADMET data can predict properties such as blood-brain barrier permeability, liver toxicity, and bioavailability [11].

Deep learning has shown significant accuracy in toxicity prediction, even outperforming traditional in vitro assays in some instances [12].

### Biomarker Discovery and Personalized Medicine

AI helps in discovering diagnostic and prognostic biomarkers by analyzing high-dimensional patient data. Integrating AI with electronic health records (EHRs) and omics data allows for the stratification of patient populations and the development of personalized therapies [13].

### Clinical Trial Design and Patient Recruitment

AI can optimize clinical trial designs by predicting patient responses and identifying suitable cohorts from EHRs and genomics databases. This improves recruitment efficiency and trial outcomes [14].

## Notable AI Platforms in Drug Discovery

**Several AI platforms have emerged as leaders in pharmaceutical R&D**

- **Atomwise:** Uses deep learning for structure-based drug design and hit discovery [15].
- **Insilico Medicine:** Applies generative adversarial networks (GANs) for target discovery and molecule generation [16].
- **Benevolent AI:** Integrates AI and bioscience data to propose drug candidates and repurposing opportunities [17].
- **DeepMind (AlphaFold):** Accurately predicts protein structures, aiding in understanding drug-target interactions [18].

## Case Studies

### Exscientia – DSP-1181

Exscientia, in collaboration with Sumitomo Dainippon Pharma, developed DSP-1181, a serotonin 5-HT1A receptor agonist for obsessive-compulsive disorder (OCD), using AI-based drug design. It took just 12 months from target selection to preclinical trials—much shorter than the average timeline [19].

### Baricitinib for COVID-19

BenevolentAI used its knowledge graph to identify baricitinib, an existing rheumatoid arthritis drug, as a potential treatment for COVID-19. It was later validated in clinical trials and authorized for emergency use by the FDA [20].

## Challenges and Limitations

**Despite its promise, AI in drug discovery faces several challenges**

### Data Quality and Availability

AI models require large, high-quality datasets. Incomplete, inconsistent, or biased data can lead to poor predictions [21]. Moreover, much valuable data is proprietary and not publicly accessible.

### Interpretability of Models

Deep learning models often function as "black boxes," making it difficult to interpret how predictions are made. This limits trust among regulatory bodies and scientists [22].

### Regulatory Hurdles

Regulatory frameworks are still evolving to address the use of AI in drug development. Demonstrating reproducibility, robustness, and safety of AI-derived predictions is critical for approval [23].

### Integration with Experimental Workflows

AI tools must be integrated with wet-lab experiments, requiring collaboration between computational scientists and experimental pharmacologists. Misalignment between in silico and in vitro results can reduce efficiency [24].

## Future Perspectives

The future of drug discovery is anticipated to be more data-driven and patient-centric, with AI playing a central role. Key developments expected include:

- **Integration of Multi-Omics Data:** AI will help integrate genomics, transcriptomics, proteomics, and metabolomics data for holistic understanding of diseases and drugs.
- **Federated Learning:** Preserves data privacy while enabling AI models to learn from decentralized datasets [25].
- **Explainable AI (XAI):** Will help in building interpretable and trustworthy models.
- **Quantum Computing + AI:** May drastically enhance computational drug discovery by simulating molecular interactions at quantum levels [26].

## Conclusion

AI and ML are transforming drug discovery by enhancing speed, accuracy, and cost-effectiveness. From target identification to clinical trials, these technologies enable novel insights and predictive capabilities previously unattainable through conventional approaches. While challenges remain, ongoing advances in algorithms, data

curation, and interdisciplinary collaboration are steadily addressing these barriers. As regulatory agencies adapt to technological shifts, the fusion of AI with pharmaceutical R&D is poised to bring about a new era of precision medicine and rapid therapeutic innovation.

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Both Authors contributed equally

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