



Artificial Intelligence–Driven Drug Discovery: Transforming Modern Drug Development

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Abstract

Artificial intelligence (AI) has emerged as an important technology in modern drug discovery, enabling researchers to analyze complex chemical and biological datasets and accelerate the identification of promising therapeutic candidates. Conventional drug discovery is often associated with high costs, lengthy development timelines, extensive experimental screening, and high attrition rates. Machine learning, deep learning, graph neural networks, generative models, and other AI approaches are increasingly being applied to target identification, virtual screening, molecular property prediction, drug–target interaction analysis, de novo molecular design, ADMET prediction, drug repurposing, and synthesis planning. Recent developments in three-dimensional molecular modeling and biomolecular structure prediction have further expanded the potential of AI in medicinal chemistry. However, challenges involving data quality, model interpretability, generalizability, reproducibility, and experimental validation remain. This mini-review summarizes key applications of AI in drug discovery, discusses its major advantages and limitations, and highlights future opportunities for integrating AI with medicinal chemistry and experimental research.

Keywords: Artificial intelligence; drug discovery; medicinal chemistry; machine learning; deep learning; generative AI; virtual screening; molecular docking; QSAR; ADMET

Abbreviations

AI: Artificial Intelligence; ML: Machine Learning; DL: Deep Learning; GNNs: Graph Neural Networks; ADMET: Absorption, Distribution, Metabolism, Excretion, and Toxicity.

Introduction

The discovery of new therapeutic agents is a complex process involving target identification, hit discovery, lead optimization, preclinical evaluation, and clinical development. Conventional drug discovery depends extensively on experimental screening and iterative chemical optimization. Although this approach has produced many

successful medicines, it requires considerable time, financial resources, and laboratory effort. The increasing availability of chemical, biological, genomic, proteomic, and structural datasets has created opportunities for computational approaches to complement conventional drug discovery [1,2].

Artificial intelligence (AI), particularly machine learning (ML) and deep learning (DL), is increasingly being incorporated into pharmaceutical research. AI models can identify relationships between molecular structures, biological targets, and experimental measurements, allowing researchers to predict molecular properties and prioritize compounds before extensive laboratory testing [1,3]. Recent

advances in graph neural networks (GNNs), generative models, transformers, and three-dimensional molecular modeling have expanded AI applications from prediction toward molecular design [4-7].

AI is therefore becoming an important tool in modern medicinal chemistry. However, its greatest value is likely to arise through integration with experimental research rather than replacement of medicinal chemists and laboratory scientists.

AI Technologies in Drug Discovery

Several computational approaches contribute to AI-driven drug discovery. Traditional ML methods, including random forests, support vector machines, and gradient-boosting algorithms, have been used for biological activity, toxicity, pharmacokinetic, and drug-likeness prediction [1,2].

Deep learning can identify complex relationships from large datasets. GNNs are particularly useful for medicinal chemistry because molecules can be represented as graphs consisting of atoms and chemical bonds. These models have applications in molecular property prediction, virtual screening, and drug-target interaction analysis [4].

Three-dimensional molecular representation is another important development. AI models such as Uni-Mol incorporate three-dimensional structural information and can be used for molecular property and interaction-related prediction tasks [7].

Generative AI represents a major shift from predicting existing molecules toward designing new ones. Generative models can propose molecules according to desired properties such as potency, selectivity, solubility, and synthetic accessibility. Transformers and diffusion-based models are increasingly being investigated for this purpose [5,6].

Applications of AI in Drug Discovery

Target Identification

AI can analyze genomic, proteomic, transcriptomic, clinical, and literature-derived datasets to identify potential therapeutic targets. Machine-learning models can prioritize disease-associated genes and proteins and identify relationships between molecular pathways and disease phenotypes [1,3]. This approach is particularly useful for complex diseases involving multiple biological mechanisms. Nevertheless, computationally identified targets require experimental validation to establish their biological and

therapeutic relevance.

Virtual Screening and Molecular Docking

Virtual screening is used to identify promising compounds from large chemical libraries. AI can improve compound prioritization by learning molecular and protein-ligand interaction patterns. Deep-learning approaches such as EquiBind and DiffDock have demonstrated the potential of geometric and diffusion-based models for predicting ligand-binding structures and docking poses [4,8].

AI-assisted screening can reduce the number of compounds requiring experimental testing. However, prediction accuracy can depend on the quality of training data, protein flexibility, target characteristics, and differences between computational and experimental conditions.

QSAR and Molecular Property Prediction

Quantitative structure-activity relationship (QSAR) modeling is an established method for relating molecular structure to biological activity. Modern AI and deep-learning approaches have expanded QSAR by enabling more complex molecular representations to be analyzed [1,2].

AI models can predict biological activity, solubility, lipophilicity, permeability, metabolic stability, toxicity, and other drug-related properties. Such predictions can help medicinal chemists prioritize compounds before synthesis and biological testing. However, models trained on limited chemical space may perform poorly when applied to novel molecular scaffolds, making external validation important.

De Novo Molecular Design

Generative AI is one of the most promising applications of AI in medicinal chemistry. Instead of optimizing only existing molecules, generative models can propose new chemical structures with selected properties. Deep-learning approaches have demonstrated the ability to generate novel biologically active compounds, including inhibitors of therapeutic targets [10].

Modern generative systems can simultaneously consider potency, selectivity, physicochemical properties, toxicity, and synthetic accessibility [5,6]. This multi-parameter optimization is particularly attractive because successful drug candidates must satisfy several requirements simultaneously. However, computationally generated molecules still require chemical synthesis and experimental validation.

Drug-Target Interaction Prediction

AI models can predict potential interactions between small molecules and proteins using chemical structures, protein sequences, three-dimensional information, and experimental interaction datasets. GNNs and three-dimensional molecular models can learn structural characteristics associated with binding [4,7].

These approaches can support virtual screening and help prioritize compounds for experimental studies. Dataset bias and differences between experimental assays, however, can affect prediction performance.

ADMET Prediction

Absorption, distribution, metabolism, excretion, and toxicity (ADMET) properties strongly influence the success of drug candidates. AI models can predict properties such as solubility, permeability, metabolic stability, cytochrome P450 interactions, and potential toxicity.

Early ADMET prediction can help remove unsuitable candidates before expensive experimental studies. Combining ADMET prediction with generative molecular design may allow researchers to prioritize compounds with both favorable biological and pharmacokinetic characteristics. Nevertheless, computational predictions must be experimentally confirmed.

Drug Repurposing and Synthesis Planning

AI can analyze relationships among drugs, targets, diseases, and biological pathways to identify potential new therapeutic applications for existing drugs. Because repurposed drugs may already have pharmacological and safety information, AI-assisted repurposing can potentially shorten the early stages of drug development [1,3].

AI is also increasingly used in chemical synthesis planning. Transformer-based models can predict chemical reactions and assist with retrosynthetic analysis, helping researchers identify practical synthetic routes for computationally designed molecules [6].

Advantages and Challenges

AI provides several potential advantages for drug discovery, including rapid analysis of large datasets, prioritization of chemical libraries, prediction of molecular properties, acceleration of virtual screening, and generation of novel molecular structures. It can also support simultaneous optimization of several drug-like properties [1,3].

However, important challenges remain. AI models depend strongly on the quality and diversity of training data. Experimental datasets may contain missing values, inconsistent measurements, bias, and limited chemical diversity. Deep-learning models may also be difficult to interpret, making it challenging to understand why a particular prediction was produced.

Generalizability is another major concern. A model that performs well on compounds similar to its training dataset may not perform equally well on novel chemical scaffolds. Reproducibility and prospective experimental validation are therefore essential.

Most importantly, AI predictions cannot replace laboratory experiments. Predicted activity, binding, pharmacokinetics, and toxicity must ultimately be confirmed through biochemical, cellular, preclinical, and clinical studies [3].

Future Perspectives

The future of AI-driven drug discovery is likely to involve increasingly integrated and multimodal systems. Future models may combine molecular structures, protein sequences, three-dimensional structures, omics information, experimental results, scientific literature, and clinical data.

Generative AI may increasingly support multi-objective molecular design by simultaneously considering potency, selectivity, ADMET properties, safety, and synthetic accessibility [5]. AI may also become increasingly integrated with automated laboratories, creating iterative workflows in which computational systems propose molecules, automated platforms synthesize and test them, and experimental results are used to guide subsequent molecular design.

Human expertise will remain essential. Medicinal chemists provide knowledge concerning chemical feasibility, structure-activity relationships, biological mechanisms, and experimental interpretation that may not be captured by computational datasets. Therefore, the most promising future model is AI-augmented drug discovery, in which AI accelerates prediction and exploration while scientists provide validation and decision-making.

Conclusion

Artificial intelligence is transforming modern medicinal chemistry by providing powerful approaches for target identification, virtual screening, molecular property prediction, molecular docking, de novo molecular design, ADMET prediction, drug repurposing, and synthesis

planning. Advances in deep learning, graph neural networks, generative AI, and three-dimensional molecular modeling have expanded the role of computational methods throughout the drug discovery pipeline. Nevertheless, data quality, interpretability, generalizability, reproducibility, and experimental validation remain important challenges. AI should therefore be regarded as a complementary technology rather than a replacement for experimental research. Continued integration of AI with medicinal chemistry expertise and high-quality experimental data may enable faster, more efficient, and more rational discovery of future therapeutic agents.

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