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ARTIFICIAL INTELLIGENCE–DRIVEN DRUG DISCOVERY: ACCELERATING LEAD IDENTIFICATION AND OPTIMIZATION

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Abstract

The traditional drug discovery process is characterized by high financial costs, long development timelines, and substantial rates of failure during preclinical and clinical evaluation. Recent advances in artificial intelligence (AI) have introduced new computational approaches capable of transforming multiple stages of pharmaceutical research, particularly target identification, virtual screening, lead discovery, molecular optimization, and prediction of pharmacokinetic and toxicological properties. Machine learning, deep learning, generative artificial intelligence, graph neural networks, and natural language processing enable the rapid analysis of large-scale biological, chemical, genomic, and clinical datasets that would otherwise be difficult to evaluate using conventional methods. AI-driven platforms can identify complex molecular patterns, predict drug–target interactions, generate novel chemical structures, and optimize promising compounds according to potency, selectivity, safety, and drug-like properties. These technologies therefore have the potential to reduce the number of compounds requiring experimental screening and improve the efficiency of lead identification and optimization. However, several challenges remain, including data quality, model interpretability, reproducibility, algorithmic bias, regulatory acceptance, and the need for experimental validation. This article examines the role of artificial intelligence in modern drug discovery with particular emphasis on its application in accelerating lead identification and lead optimization. It also discusses major AI methodologies, their integration with traditional pharmaceutical research, current limitations, and future perspectives for the development of safer and more effective therapeutic agents.

Keywords: artificial intelligence, drug discovery, machine learning, deep learning, lead identification, lead optimization, virtual screening, drug–target interaction, molecular design, generative AI, pharmacokinetics, toxicity prediction.

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Introduction

Drug discovery is a complex, multidisciplinary, and resource-intensive process that involves the identification of biologically relevant targets, discovery of active chemical compounds, optimization of lead molecules, preclinical investigation, and subsequent clinical development. Despite significant advances in molecular biology, medicinal chemistry, pharmacology, and biotechnology, the development of a new therapeutic agent continues to require substantial financial investment and many years of research. One of the major challenges associated with conventional drug discovery is the high attrition rate of candidate compounds. Many molecules that demonstrate promising activity during early laboratory investigations fail during later stages because of insufficient efficacy, unfavorable pharmacokinetic characteristics, toxicity, poor bioavailability, or unexpected biological interactions.Traditional approaches to drug discovery have largely depended on experimental screening, medicinal chemistry expertise, structure–activity relationship studies, and iterative synthesis and testing of numerous chemical compounds. Although these approaches remain essential, they can be time-consuming and expensive, particularly when researchers are required to evaluate extremely large chemical libraries. Modern pharmaceutical databases contain millions to billions of potential molecular structures, making comprehensive experimental screening practically impossible. Consequently, computational methods have become increasingly important for identifying compounds with the greatest probability of biological activity before experimental validation.

Artificial intelligence has emerged as one of the most promising technologies for addressing these limitations. AI refers to computational systems capable of performing tasks that traditionally require human intelligence, including pattern recognition, prediction, classification, optimization, and decision support. Within pharmaceutical research, AI encompasses several computational techniques, including machine learning, deep learning, artificial neural networks, graph neural networks, reinforcement learning, natural language processing, and generative modeling. These methods can process large and heterogeneous datasets and identify relationships that may not be apparent through conventional statistical analysis.Machine learning algorithms are particularly valuable in drug discovery because they can learn relationships between molecular structures and experimentally observed biological activities. When trained using sufficiently reliable datasets, these models can predict whether a new compound is likely to interact with a particular biological target. Such predictions can significantly reduce the number of molecules that require laboratory testing. Instead of experimentally screening millions of compounds, researchers can use AI-based models to prioritize a smaller group of candidates with favorable predicted activity.

Deep learning has further expanded the capabilities of computational drug discovery. Deep neural networks can automatically identify complex patterns within chemical and biological datasets without requiring extensive manual feature engineering. Molecular structures can be represented using fingerprints, molecular descriptors, graphs, strings, or three-dimensional structural information. AI models can then analyze these representations to estimate biological activity, binding affinity, selectivity, solubility, membrane

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permeability, metabolic stability, and potential toxicity.One of the most important applications of artificial intelligence is **lead identification**. Lead compounds are molecules that demonstrate sufficient biological activity against a therapeutic target and possess characteristics that justify further optimization. Identifying suitable lead compounds traditionally requires high-throughput screening of large chemical libraries. AI-assisted virtual screening provides an alternative strategy in which computational models predict the probability that individual molecules will interact with a biological target. Molecules with favorable predicted properties can then be selected for experimental testing, thereby reducing laboratory workload and accelerating the discovery process.

AI may also enhance structure-based drug discovery. When the three-dimensional structure of a therapeutic target is available, computational docking and molecular modeling approaches can be combined with machine learning algorithms to estimate ligand–target interactions. AI-based scoring functions can improve the prioritization of potential ligands by considering complex structural characteristics and interaction patterns. Advances in protein structure prediction have further increased the number of biological targets that can potentially be investigated using structure-based computational methods.Another rapidly developing area is generative artificial intelligence. Generative models can design completely new molecular structures rather than selecting compounds exclusively from existing chemical libraries. These algorithms can be trained to generate molecules that satisfy specific pharmaceutical criteria, such as high binding affinity, appropriate molecular weight, improved solubility, limited toxicity, and favorable metabolic characteristics. Generative molecular design therefore expands the searchable chemical space and may enable researchers to discover novel compounds that would be unlikely to emerge through traditional screening strategies.

Artificial intelligence is equally important during **lead optimization**, the stage in which promising lead compounds are systematically modified to improve their pharmaceutical properties. A compound with strong biological activity may still be unsuitable for clinical development if it has poor absorption, rapid metabolism, inadequate tissue distribution, undesirable off-target effects, or significant toxicity. Medicinal chemists therefore modify molecular structures to achieve an optimal balance between potency and drug-like properties.AI-based quantitative structure–activity relationship models can predict how structural modifications may influence the biological activity of a molecule. Similar models may also estimate absorption, distribution, metabolism, excretion, and toxicity characteristics, commonly referred to as ADMET properties. These predictions allow researchers to identify unfavorable compounds earlier in the development process and prioritize structural modifications that are more likely to improve overall pharmacological performance.

The integration of artificial intelligence with omics technologies has created additional opportunities for drug discovery. Genomics, transcriptomics, proteomics, metabolomics, and other high-throughput biological technologies generate enormous amounts of information about disease-related molecular mechanisms. AI can integrate these datasets to identify disease-associated pathways, therapeutic targets, biomarkers, and potential drug

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candidates. Such approaches are particularly valuable in complex diseases in which multiple genes, proteins, and signaling pathways contribute to disease development.Natural language processing also plays an important role in pharmaceutical research. The scientific literature contains an enormous amount of information regarding biological pathways, molecular interactions, therapeutic targets, clinical outcomes, and adverse effects. Manually reviewing this literature is increasingly difficult because thousands of biomedical publications are produced continuously. NLP-based systems can extract relevant information from scientific articles, patents, clinical trial records, and pharmacological databases and organize it into structured knowledge resources. This capability may assist researchers in identifying previously overlooked relationships between diseases, targets, and therapeutic compounds.

Artificial intelligence also contributes to drug repurposing, which involves identifying new therapeutic applications for existing drugs. Because approved or previously investigated compounds already possess substantial pharmacological and safety information, successful drug repurposing may significantly reduce development time. AI algorithms can analyze molecular, genomic, clinical, and pharmacological data to identify unexpected relationships between existing medications and diseases. This approach has attracted particular attention for rare diseases and conditions in which conventional drug development may be economically or scientifically challenging.Despite the considerable potential of artificial intelligence, AI-driven drug discovery also presents several important limitations. The performance of AI models strongly depends on the quality and representativeness of the datasets used for training. Incomplete, inconsistent, biased, or incorrectly labeled data can result in unreliable predictions. Furthermore, highly complex deep learning models may operate as “black boxes,” making it difficult to understand the biological or chemical basis of individual predictions. Model interpretability is especially important in pharmaceutical research because scientific and regulatory decisions require transparent and reproducible evidence.

Another significant limitation is the difference between computational prediction and biological reality. A molecule predicted to have excellent properties by an AI system may fail during experimental testing because biological systems involve complex interactions that are difficult to model completely. Consequently, artificial intelligence should not be considered a replacement for experimental pharmacology, medicinal chemistry, or clinical research. Instead, AI should function as a complementary decision-support technology that helps researchers identify the most promising hypotheses and candidate molecules for further investigation.The increasing integration of AI with laboratory automation, high-throughput experimentation, structural biology, cloud computing, and large biomedical databases is expected to create increasingly efficient drug discovery pipelines. In such systems, AI algorithms can propose new molecular structures, automated platforms can synthesize and test them, and the resulting experimental data can be returned to computational models for further optimization. This iterative process may substantially shorten traditional design–synthesis–test–analysis cycles.

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Therefore, artificial intelligence represents a major technological development in contemporary pharmaceutical research. Its capacity to analyze enormous datasets, predict molecular behavior, prioritize lead compounds, design novel chemical structures, and optimize pharmacological properties has the potential to improve both the speed and efficiency of drug development. The present study focuses on the application of artificial intelligence in lead identification and optimization and evaluates how AI-based technologies can contribute to the development of more effective, selective, and safer therapeutic candidates.

Materials and Methods

This study used a narrative review approach to evaluate the application of artificial intelligence in drug discovery, with particular attention to lead identification and lead optimization. Scientific publications related to machine learning, deep learning, virtual screening, molecular docking, generative models, drug–target interaction prediction, and ADMET assessment were analyzed. Relevant information was collected from peer-reviewed articles, biomedical databases, and pharmaceutical research literature. The selected studies were compared according to their use of AI algorithms, molecular datasets, prediction methods, and reported outcomes. Particular emphasis was placed on how artificial intelligence can reduce the number of compounds requiring experimental screening, improve the prediction of biological activity, and support the optimization of pharmacokinetic and safety properties. The collected information was synthesized to identify the main advantages, current limitations, and practical applications of AI-driven approaches in modern drug discovery.

Results

The analysis showed that artificial intelligence has become an increasingly important component of modern drug discovery, particularly in the identification and optimization of lead compounds. Across the reviewed applications, AI-based methods demonstrated strong potential to improve the efficiency of compound screening, predict molecular behavior, and reduce the number of candidates that require extensive experimental evaluation. Machine learning and deep learning approaches were especially useful for processing large chemical and biological datasets and identifying relationships between molecular structure, biological activity, and pharmacological properties.One of the most important findings was the effectiveness of AI-assisted virtual screening. Conventional high-throughput screening requires the experimental testing of a large number of compounds, whereas AI-based virtual screening can prioritize molecules according to their predicted probability of interacting with a selected biological target. This approach enables researchers to focus laboratory resources on a smaller group of candidates with higher predicted activity. Machine learning models can analyze molecular descriptors, chemical fingerprints, structural features, and previously reported activity data to classify or rank candidate compounds. As a result, potentially inactive compounds may be excluded before expensive experimental procedures are performed.

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Deep learning techniques were found to provide additional advantages in the analysis of highly complex molecular data. Neural network-based systems can process multiple types of information, including chemical structures, protein sequences, three-dimensional molecular conformations, and biological assay results. These models are capable of identifying nonlinear relationships that may be difficult to detect using conventional computational approaches. Their application may therefore improve the prediction of binding affinity, biological activity, and compound selectivity during early-stage drug discovery.Another major area identified was AI-supported prediction of drug–target interactions. Determining whether a small molecule can effectively interact with a specific protein or receptor is essential for lead identification. AI models can integrate molecular characteristics of both compounds and biological targets to estimate the likelihood and strength of these interactions. When combined with molecular docking and structural modeling, these approaches can help identify candidate molecules that demonstrate favorable interactions within the binding site of a therapeutic target. Such integration may improve the selection of lead compounds for subsequent experimental validation.

The reviewed approaches also demonstrated an important role for generative artificial intelligence in molecular design. Unlike traditional virtual screening, which evaluates compounds from existing chemical libraries, generative models can propose entirely new molecular structures. These systems may be optimized to generate molecules with predefined characteristics, including high predicted target affinity, appropriate molecular size, improved solubility, acceptable lipophilicity, and reduced toxicity. Generative AI therefore expands the available chemical space and offers a strategy for producing novel candidate molecules that may not already exist in conventional compound databases.

Artificial intelligence was also shown to be particularly valuable during the lead optimization stage. After a promising compound is identified, its structure must frequently be modified to improve potency, selectivity, pharmacokinetic characteristics, and safety. AI-based quantitative structure–activity relationship models can predict how individual structural changes may alter biological activity. This allows researchers to compare multiple molecular modifications computationally before synthesizing each new compound. Consequently, medicinal chemists may prioritize structural modifications that are more likely to produce favorable pharmacological profiles.The prediction of absorption, distribution, metabolism, excretion, and toxicity properties was another important application identified in the analysis. A molecule with strong activity against a therapeutic target may still fail as a drug candidate if it has poor bioavailability, unfavorable metabolism, low tissue penetration, or significant toxicity. AI-based ADMET prediction models can estimate these properties at an early stage of development. Early identification of compounds with unfavorable characteristics may reduce the risk of investing extensive resources in candidates that are unlikely to progress successfully through later stages of drug development.

The analysis further indicated that AI can support multi-parameter optimization. Drug candidates must satisfy several requirements simultaneously, including biological potency, target selectivity, chemical stability, solubility, permeability, metabolic stability, and

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acceptable toxicity. Improving one property may sometimes negatively affect another. AI-based optimization methods can evaluate multiple parameters simultaneously and assist researchers in identifying compounds with the most balanced overall profile. This capability is particularly important in lead optimization, where the objective is not merely to maximize biological activity but to achieve a combination of characteristics compatible with successful drug development.Artificial intelligence also demonstrated value in the analysis of large-scale biological datasets. Genomic, transcriptomic, proteomic, and metabolomic data can be integrated to provide a more comprehensive understanding of disease mechanisms and potential therapeutic targets. AI algorithms can identify complex patterns within these datasets and help determine which molecular pathways or proteins may represent promising intervention points. Such analyses may contribute indirectly to lead identification by improving target selection and enabling the development of compounds against biologically relevant mechanisms.

Natural language processing was another useful AI application identified in pharmaceutical research. NLP-based systems can analyze large volumes of scientific literature, patents, clinical trial information, and pharmacological databases. These tools can extract information about molecular interactions, disease mechanisms, therapeutic targets, adverse effects, and previously investigated compounds. This can help researchers identify relevant evidence more efficiently and may support the discovery of relationships that are difficult to recognize through manual literature review.

AI-based methods also showed potential in drug repurposing. By comparing molecular targets, disease pathways, gene-expression profiles, and known drug effects, computational models can identify existing compounds that may have therapeutic activity in diseases for which they were not originally developed. Although repurposing differs from the development of completely new chemical entities, this approach may shorten some stages of discovery because important information about the pharmacology and safety of existing drugs may already be available.Despite these advantages, the analysis also highlighted important limitations. The accuracy of AI-based predictions depends strongly on the quality, completeness, and diversity of the training data. Models trained using limited or biased datasets may produce unreliable results when applied to new chemical structures or biological targets. In addition, complex deep learning models may provide predictions without clearly explaining the molecular features responsible for those predictions. Limited interpretability may reduce confidence in AI-based decisions and make experimental validation particularly important.

Another limitation is that computational predictions cannot fully reproduce the complexity of living biological systems. Drug activity may be influenced by factors such as metabolism, tissue distribution, protein binding, compensatory signaling pathways, immune responses, and individual biological variability. Therefore, promising AI predictions must be confirmed through in vitro and in vivo experiments before clinical development. The results indicate that the greatest value of artificial intelligence lies in supporting and accelerating experimental decision-making rather than completely replacing laboratory research.Overall, the findings suggest that AI-driven approaches can strengthen

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the drug discovery pipeline by enabling faster screening of chemical space, more efficient identification of promising lead compounds, improved prediction of molecular properties, and more systematic lead optimization. The combination of machine learning, deep learning, generative models, molecular docking, and ADMET prediction provides a computational framework that can assist researchers throughout multiple stages of early drug development.

Table 1. Major applications of artificial intelligence in drug discovery

AI application	Main function	Role in drug discovery	Potential benefit
Virtual screening	Computational evaluation of large compound libraries	Lead identification	Prioritizes promising molecules before laboratory testing
Machine learning	Prediction based on molecular descriptors and activity data	Lead identification and optimization	Reduces unnecessary experimental screening
Deep learning	Analysis of complex chemical and biological patterns	Activity and property prediction	Improves recognition of nonlinear molecular relationships
Drug–target interaction prediction	Estimation of compound–protein interactions	Lead selection	Helps identify candidates with favorable target affinity
Molecular docking	Assessment of ligand binding to target structures	Structure-based discovery	Supports prioritization of compounds according to predicted binding
Generative AI	Creation of novel molecular structures	De novo drug design	Expands chemical space and generates optimized candidates
QSAR modeling	Prediction of structure–activity relationships	Lead optimization	Guides structural modification of candidate molecules
ADMET prediction	Estimation of pharmacokinetic and toxicological properties	Lead optimization	Supports early elimination of unsuitable compounds
Multi-parameter optimization	Simultaneous evaluation of multiple molecular properties	Lead optimization	Improves balance between potency, selectivity, and drug-like properties

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AI application	Main function	Role in drug discovery	Potential benefit
Natural language processing	Extraction of information from scientific and clinical literature	Knowledge discovery	Accelerates identification of relevant targets and compounds
AI-assisted drug repurposing	Identification of new uses for existing drugs	Therapeutic discovery	May reduce some stages of development

Discussion

The findings of this study indicate that artificial intelligence has the potential to substantially transform the conventional drug discovery process by improving both lead identification and lead optimization. Traditional drug discovery frequently involves the screening of very large compound libraries, repeated synthesis of chemical analogues, and extensive biological testing. These procedures are scientifically valuable but require considerable time, financial resources, and laboratory capacity. AI-based approaches offer a complementary strategy by prioritizing the most promising compounds before experimental testing and by predicting how structural modifications may influence biological activity and pharmacological properties.One of the most significant advantages of AI is its ability to analyze large and heterogeneous datasets. Modern pharmaceutical research generates substantial amounts of information from chemical libraries, biological assays, genomic studies, protein databases, clinical trials, and published scientific literature. Conventional analytical methods may struggle to integrate such diverse data. Machine learning and deep learning systems can identify complex relationships among these datasets and generate predictions that may support more informed decisions during early drug development. In this context, AI does not simply increase computational speed; it also provides a method for detecting molecular patterns that may otherwise remain unrecognized.

Virtual screening represents one of the most practical applications of AI in lead identification. Rather than experimentally testing every molecule, researchers can use predictive models to rank compounds according to their estimated probability of interacting with a therapeutic target. This can significantly narrow the number of compounds selected for biological evaluation. The major benefit of this approach is the more efficient allocation of laboratory resources. However, the quality of virtual screening results depends heavily on the accuracy of the molecular representations, the characteristics of the training dataset, and the biological relevance of the selected target.Deep learning has expanded the analytical capacity of AI-based drug discovery because it can process complex representations of molecules and proteins. Graph-based models are particularly relevant because molecular structures can naturally be represented as graphs composed of atoms and chemical bonds. Such representations may preserve structural information more effectively than simplified molecular descriptors. At the same time, deep learning models often require large, well-curated datasets, and their internal decision-making mechanisms

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can be difficult to interpret. Therefore, improved prediction performance should be balanced with the need for transparency and biological explainability.

Generative AI represents a further shift in drug discovery because it can move beyond screening existing chemical libraries and instead design new molecules. Generative models can be trained to propose structures with desired features, such as high target affinity, improved solubility, reduced toxicity, and appropriate physicochemical properties. This approach may broaden the range of candidate molecules available to medicinal chemists. Nevertheless, generated compounds must still be chemically feasible, synthesizable, stable, and biologically active. For this reason, generative AI is most effective when combined with medicinal chemistry expertise and experimental validation.Lead optimization is another area in which AI may provide considerable value. During this stage, researchers attempt to improve multiple properties simultaneously, including potency, selectivity, solubility, metabolic stability, bioavailability, and safety. These objectives are often interconnected, and improvement of one property may negatively affect another. AI-based multi-parameter optimization can help researchers evaluate these trade-offs and prioritize molecular modifications that produce a more balanced pharmacological profile. This could reduce the number of iterative synthesis cycles required during conventional medicinal chemistry optimization.

The prediction of ADMET properties is especially important because many drug candidates fail due to unfavorable pharmacokinetic or toxicological characteristics rather than insufficient activity against the intended target. AI-based models may identify such problems at an earlier stage and therefore reduce unnecessary progression of unsuitable compounds. Early prediction of absorption, metabolism, toxicity, and related parameters may improve the efficiency of candidate selection. However, these predictions should be treated as supportive evidence rather than definitive proof, because in vivo pharmacokinetics and toxicity are influenced by complex biological mechanisms that remain difficult to model completely.Another important consideration is the quality of data used to train AI systems. Drug discovery datasets can contain incomplete information, inconsistent experimental conditions, measurement errors, and strong representation biases toward well-studied targets or chemical classes. An AI model trained on such data may achieve high performance within its original dataset but perform poorly when applied to structurally different molecules or new biological systems. External validation and independent experimental testing are therefore essential for establishing the generalizability of AI-based predictions.

Model interpretability is also becoming increasingly important. In pharmaceutical research, researchers need to understand not only what a model predicts but also why it produces a particular prediction. Explainable AI approaches may help identify molecular substructures, biological features, or interaction patterns that influence the model's output. Such information can improve scientific confidence, facilitate medicinal chemistry decisions, and support regulatory evaluation. The development of more interpretable AI systems may therefore become a major priority in future pharmaceutical research.

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AI-assisted drug discovery also benefits from integration with structural biology. The increasing availability of experimentally determined and computationally predicted protein structures has created new opportunities for structure-based drug design. When accurate target structures are available, AI can support docking, binding-site analysis, ligand generation, and affinity prediction. Combining structural information with machine learning may improve the identification of compounds that interact selectively with disease-relevant targets.The use of natural language processing adds another important dimension to AI-based drug discovery. Scientific knowledge is distributed across millions of journal articles, patents, reports, and clinical trial records. NLP tools can extract relevant information from these sources and organize relationships among drugs, targets, pathways, diseases, and adverse effects. This may assist researchers in identifying previously reported evidence, avoiding unnecessary duplication, and generating new hypotheses from existing knowledge.

Despite rapid technological development, AI should not be considered a substitute for experimental science. Computational predictions may guide researchers toward promising molecules, but the biological activity, safety, and therapeutic relevance of these molecules must ultimately be confirmed experimentally. In vitro studies, animal models when appropriate, and clinical trials remain essential stages of drug development. The most realistic model for the future is therefore a hybrid system in which AI and laboratory research continuously support each other.The integration of AI with automated synthesis and high-throughput experimentation may further accelerate this process. In a closed-loop system, AI models can propose new compounds, automated platforms can synthesize and test them, and the resulting experimental data can be used to update the computational models. This iterative design–make–test–learn approach may shorten the optimization cycle and improve the efficiency of pharmaceutical research.

From a broader perspective, AI-driven drug discovery may contribute to the development of more personalized and targeted therapies. By integrating molecular, genomic, and clinical information, AI systems may help identify patient subgroups that are more likely to respond to specific therapies. Such approaches could support precision medicine and the development of treatments tailored to particular molecular characteristics of disease.However, ethical and regulatory questions must also be considered. AI-based decisions should be transparent, reproducible, and based on high-quality data. Regulatory authorities may require clear evidence regarding model validation, data provenance, and prediction reliability before AI-generated evidence is used to support critical drug development decisions. Standardized reporting guidelines and validation frameworks will therefore be important for the wider adoption of AI technologies in pharmaceutical research.Overall, the results support the view that artificial intelligence can enhance the efficiency of modern drug discovery by accelerating lead identification, guiding molecular optimization, improving early prediction of ADMET characteristics, and supporting data-driven decision-making. Its greatest value is likely to emerge through integration with medicinal chemistry, pharmacology, structural biology, and experimental validation. As computational methods continue to improve, AI is expected to become an increasingly

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important component of the drug discovery pipeline, while the reliability of its predictions will continue to depend on rigorous data quality, validation, and biological confirmation.

Conclusion

Artificial intelligence is becoming an important component of modern drug discovery and has considerable potential to accelerate both lead identification and lead optimization. Machine learning, deep learning, graph-based neural networks, generative models, molecular docking, and AI-assisted ADMET prediction enable researchers to analyze large chemical and biological datasets, identify promising compounds, and predict important molecular properties before extensive experimental testing. These approaches can reduce unnecessary screening and support more efficient selection of drug candidates.The application of AI is particularly valuable during lead optimization, where several pharmacological and physicochemical characteristics must be considered simultaneously. Computational models can assist in predicting biological potency, target selectivity, solubility, metabolic stability, pharmacokinetic behavior, and toxicity. Generative AI further extends this potential by enabling the design of new molecular structures with predefined characteristics. Advances in protein structure prediction and structure-based computational methods have also created new opportunities for AI-assisted molecular design.However, the effectiveness of AI depends strongly on data quality, appropriate model validation, interpretability, and experimental confirmation. Computational predictions cannot completely reproduce the complexity of biological systems, and promising AI-generated candidates must therefore undergo rigorous in vitro, in vivo, and ultimately clinical evaluation. Artificial intelligence should consequently be regarded as a complementary decision-support technology rather than a replacement for medicinal chemistry, pharmacology, and experimental research.Future progress is expected to depend on the integration of artificial intelligence with high-throughput screening, automated chemical synthesis, multi-omics technologies, structural biology, and laboratory automation. Closed-loop design–make–test–learn systems may further accelerate the optimization of candidate molecules by continuously integrating experimental results into computational models. Overall, AI-driven drug discovery offers a promising strategy for improving the speed, efficiency, and precision of pharmaceutical research and may contribute to the development of safer and more effective therapeutic agents.

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