

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT TRANSFORMING MODERN PHARMACEUTICAL RESEARCH

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Abstract

Background: The pharmaceutical industry is increasingly leveraging the power of artificial intelligence (AI) to enhance drug discovery and development processes. Artificial intelligence (AI) technology is quickly revolutionizing pharmaceutical research by streamlining drug development and discovery. AI-driven drug discovery offers advanced predictions, molecular design, and data-driven decision-making, with high efficacy and fewer failures, compared to the traditional process, which is time-consuming and expensive.

Aim: This study was conducted to assess the applications, development and advancement of AI, challenges faced and future opportunities in drug discovery and development in the current scenario.

Method: A systematic literature review was carried out, based on the PRISMA 2020 framework. Studies published between 2021 and 2026 were searched for, using the databases: PubMed, Scopus, Web of Science, and Embase. Twenty-five articles were selected for qualitative synthesis following screening and eligibility criteria.

Results: The results showed that AI played a major role in various aspects of target identification, protein structure prediction, molecular generation, virtual screening, and antimicrobial discovery, drug repurposing and early clinical translation. With the help of generative AI and deep learning models, compound optimization was enhanced and promising therapeutic candidates were identified quicker. There were still data quality, model interpretability, model validation and regulatory acceptance concerns, however.

Conclusion: AI is versatile and a great tool to speed up the process of drug discovery. While it cannot be a substitute for experimental & clinical

validation, AI complements the biological research, and can help to discover safer and effective drugs.

INTRODUCTION

Pharmaceutical research is being transformed by artificial intelligence (AI), as it enables scientists to study the biological and chemical information at a scale too difficult for conventional analysis (Tehreem et al., 2024). The choices regarding disease mechanism, therapeutic target and candidate molecules in drug discovery are uncertain and the drug development process needs proof that a candidate is safe and effective. Machine learning can assist these decisions by

learning the relationships between input (x) (e.g., a protein sequence, molecular structure) and outcome (y) (e.g., the binding affinity, biological activity). A predictive model in its simplified form is the prediction $y = f_{\theta}(x)$. Where, θ the parameters θ are learned from the data. One of the most significant early advances made were the development of AlphaFold's ability to predict the structure of proteins from their amino

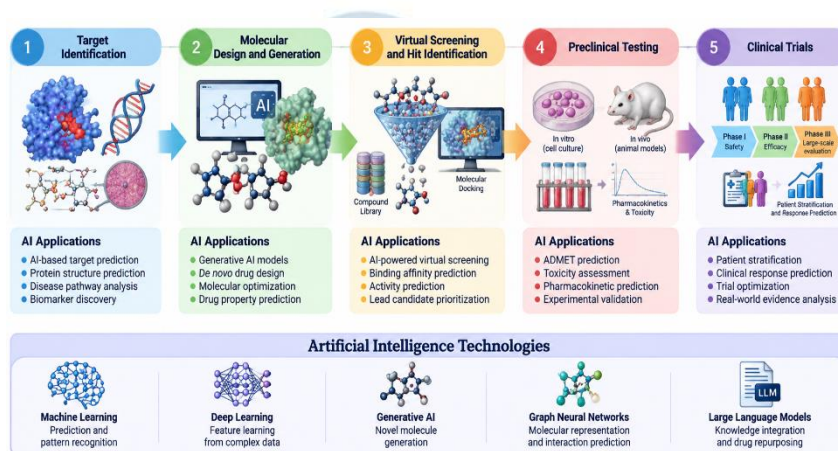


Figure 1: Artificial Intelligence-Driven Drug Discovery and Development Pipeline

acid sequences (Jumper et al., 2021; Rahman et al., 2024; Ayaz et al., 2025; Rahman et al., 2025). This could be applied to the human proteome to vastly increase the amount of information available for studying potential targets (Tunyasuvunakool et al., 2021; Batool et al., 2023; Mujeeb et al., 2025; Ashraf et al., 2025). Meanwhile, deep generative models and molecular

dynamics simulations were used, 2023d to suggest and test routes for antimicrobial peptides (AMP) (Das et al., 202; Qayyum et al., 2025). These studies set the stage for the application of AI across the whole process of therapeutic discovery (Figure 1).

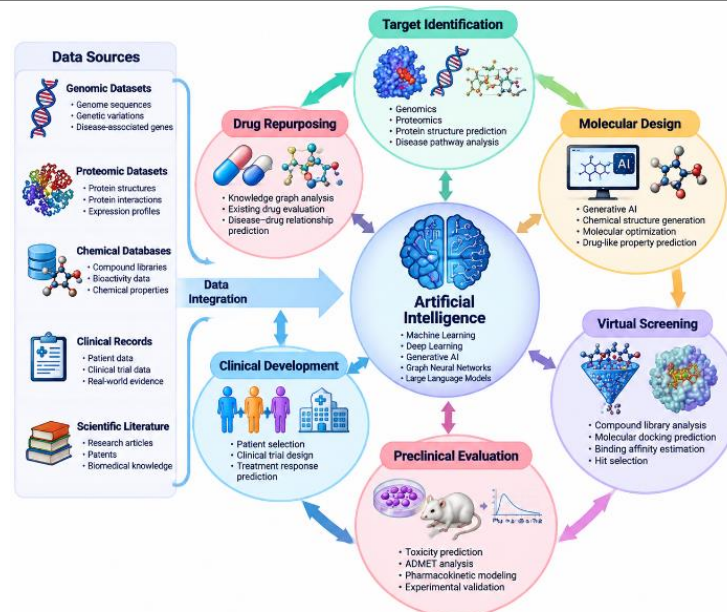


Figure 2: Integration of Artificial Intelligence across the Drug Discovery Workflow

With the maturation of the field, AI techniques were not only used to predict known properties of molecules, but also to explore molecules and enhance them for specific applications. Large-scale molecular representations demonstrated that patterns of chemical features could be learned from a large collection of unlabeled molecules, which could be utilized for property prediction or for generating new molecules that possess similar properties (Al-Kubaisi et al., 2021; Ross et al., 2022; Batool & Lashari 2025). Generative deep learning was also used to discover a powerful and selective inhibitor for RIPK1 (Li et al., 2022; Hashmi et al., 2025) and machine learning was leveraged to tune the affinity and specificity of

therapeutic antibodies (Makowski et al., 2022; Qadeer & Batool et al., 2024; Akram et al., 2024). The tasks are representative of the major challenge in drug design, that of a molecule having to simultaneously satisfy multiple requirements. Selection of candidates can be stated conceptually as the maximization of fitness function $\max_x$, where $(S(x) = \omega_1 A(x) + \omega_2 Q(x) - \omega_3 T(x))$. Where, (A) is the desired activity, Q is other desirable qualities (such as selectivity), and T is the toxicity risk. The weights ω_1 signify research priorities but the usefulness of a predicted biological behavior has to be judged by the behavior measured in the real world (Figure 2).

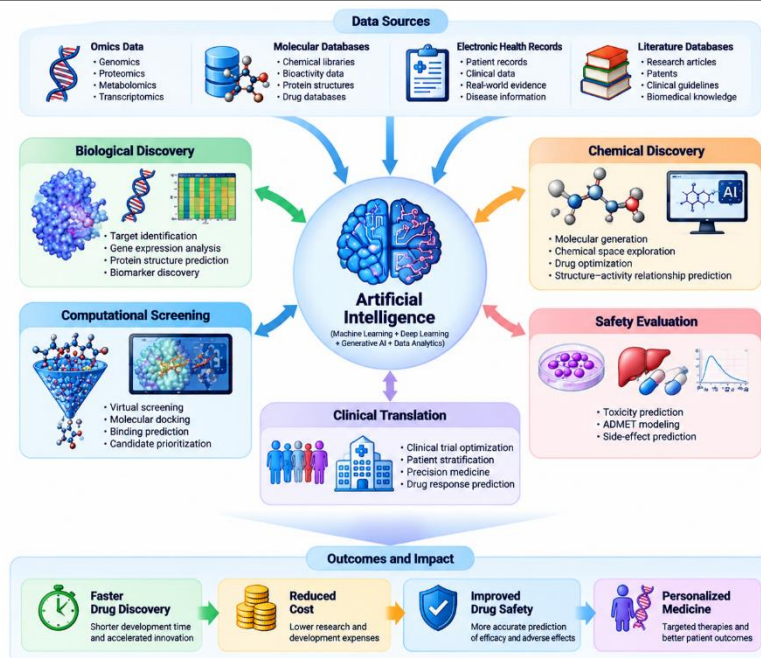


Figure 3: Role of Artificial Intelligence in Modern Pharmaceutical Research

In 2023, experiments were conducted to demonstrate the ability for AI to reduce the number of candidates in a massive search space that are worth testing. Moret et al. (2023) leveraged molecular structure and bioactivity information in chemical language models for de novo drug design. Liu et al. (2023) and Smer-Barreto et al. (2023) applied deep learning and machine learning to identify antibiotic candidates against two bacterial strains – *Acinetobacter baumannii* and *Pseudomonas aeruginosa* – and compounds with senolytic activity, respectively. These are examples of various ways in which AI can help: In the generation of molecules, AI can help identify molecules that are likely to have a desired property. In compound prioritization, AI can help prioritize compounds for experimental testing. For recognition of activity patterns from

experimental data, AI can help identify activities that are likely to be present in a given experimental dataset. Development of structural modelling then broadened the biological question which could be addressed. AlphaFold 3 predicted complexes (which include proteins, nucleic acids and small molecules) that will be helpful to study possible molecular interactions before experiments are conducted (Abramson et al., 2024). Explainable deep learning was used to identify a structural class of antibiotics, and the correlation with chemical substructures of the compounds was also achieved (Wong et al., 2024). However, a predicted structure, binding value or activity number is only a hypothesis until it can be verified with appropriate experimental data (Figure 3).

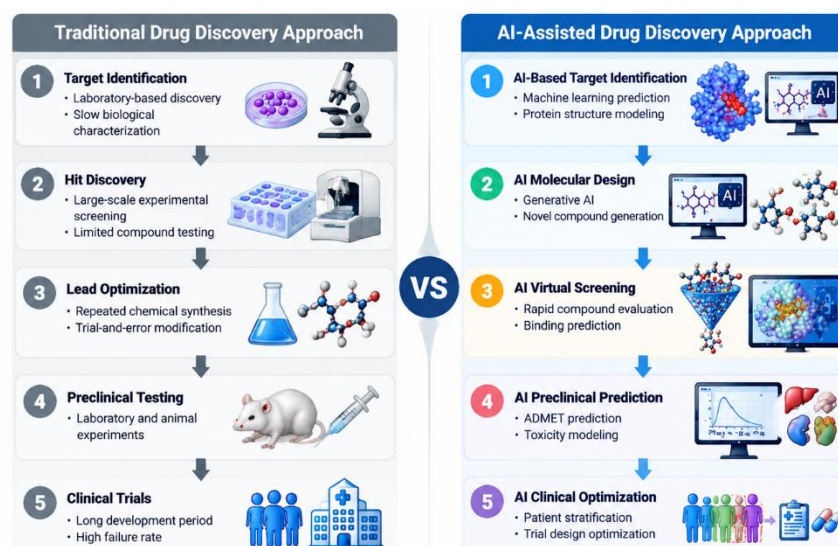


Figure 4: AI-Powered Transformation of Traditional Drug Discovery Processes

There is more recent research that has been able to expand the use of AI to target directed design, drug repurposing and finally moving towards clinical testing. Wu et al. (2024) have created a chemical language model to synthesize molecules with a particular desired purpose, and Wan et al. (2024) applied deep learning to the protein sequences from extinct organisms to identify potential antibiotic peptides. Another opportunity was explored with an opportunity recognition framework for drug repurposing that relied on existing drugs under FDA approval, but which was now being explored for new applications (Bashir et al., 2023; Huang et al., 2024). In 2025, a TNIK inhibitor was linked to the AI-driven target identification and molecular design and the study of fibrosis (Batoool et al., 2022; Ren et al., 2025). A small, preliminary trial did not provide evidence for routine clinical effectiveness, but the results of a subsequent randomized phase 2a trial of the candidate drug, identified by the AI, were encouraging and prompted further study (Xu et al., 2025). In addition, deep learning methodology was employed for finding antibiotic candidates from archaeal proteins (Torres et al., 2025). By 2026, three-dimensional generation of molecules targeting two different targets (Hamdi et al., 2023;

Su et al., 2026), experimental validation of predicted antimicrobial peptides derived from prion-related proteins (Torres et al., 2026), and AI-driven screening strategies for very large collections of molecules (Cecchini et al., 2026). The advances open up new possibilities for research and research questions, as well as a greater need to separate the performance of the technology from its established therapeutic value (Figure 4).

This background evidence suggests that the research process is connected and that the use of AI is not limited to one specific technique—predictions can inform target selection, molecular design, screening, and development—but there are new sources of uncertainty with each. A model developed using one set of data may not be as predictive of activity on other, new compounds; similarly, activity in a laboratory assay may not correlate with acceptable pharmacokinetics, safety, and clinical efficacy. The study's problem is the disconnect between the increasing use of AI in the pharmaceutical industry, and the evidence required to establish when predictions based on AI technology yield reliable results in drug discovery and development. The relevance of this study is to identify the area where the AI is

supported with experimental and/or clinical evidence and the area that needs further validation. This study aims to explore the role of AI in the modern landscape of drug discovery and development, spanning the entire spectrum from target identification, candidate generation, preclinical evaluation, and into clinical translation.

Method

The methodology followed was a systematic literature review to explore how Artificial Intelligence (AI) can contribute to the drug discovery and development process, and the impact of AI in the modern pharmaceutical research journey. To ensure transparency, reproducibility and methodological accuracy, the review was conducted using the guidelines of the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA 2020) (Page et al., 2021). Using a systematic approach, peer-reviewed research articles were searched from the main scientific databases: PubMed, Scopus, Web of Science, and Embase, between January 2021 and September 2026. A search strategy was designed by using combinations of the following keywords with the Boolean operators - ("Artificial Intelligence" OR "Machine Learning" OR "Deep Learning" OR "Generative AI" OR "Large Language Model") AND ("Drug Discovery" OR "Drug Development" OR "Molecular Design" OR "Virtual Screening" OR "Drug Repurposing" OR "Clinical Development"). Further studies that were relevant were located by hand searching the

reference lists of selected articles. The results of the search were saved in a reference management program and then duplicates were excluded prior to screening. The process of search, identification, screening, eligibility and inclusion of articles was described in a PRISMA (prioritizing sensitive research in MEDICINE) flow diagram that summarized the number of articles identified, duplicates removed, studies screened, full texts assessed, studies excluded due to eligibility issues and the number of studies finally included in the review (Page et al., 2021).

Studies were screened and selected based on the inclusion and exclusion criteria set out. Only original peer-reviewed research articles that explored the use of AI technologies in any phase of drug discovery and development - ranging from target identification through structure prediction, molecular generation, virtual screening, lead optimization, toxicity prediction, drug repurposing to clinical trial support - were included. Review articles, conference abstracts, editorials, non-peer reviewed manuscripts, and studies unrelated to pharmaceutical applications, as well as those lacking experimental and/or computational validation, were not included in the studies. Duplicates were eliminated and the titles and abstracts were then assessed for eligibility, before full-text evaluation of potentially eligible studies. The studies that were selected were analyzed and classified based on the publication year, AI methodology, therapeutic area, biological

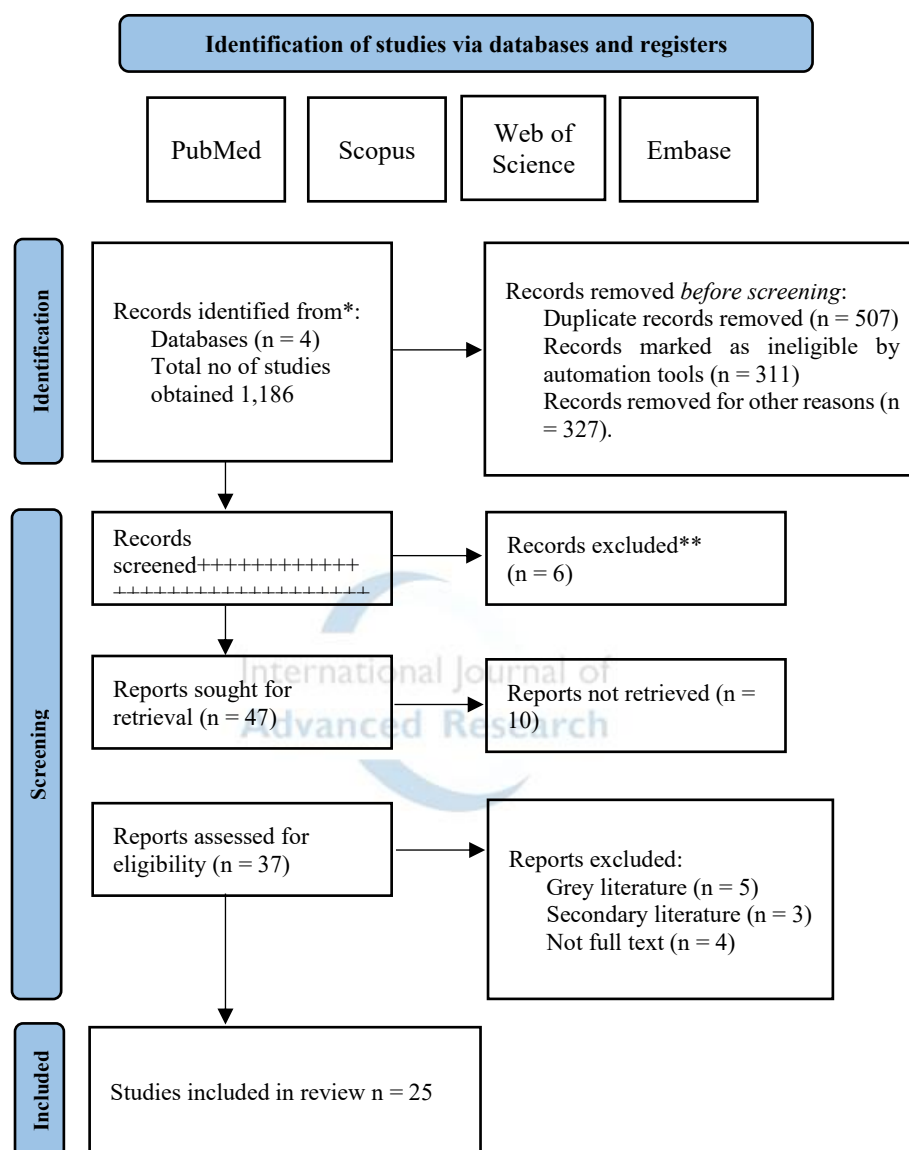


Figure 5: PRISMA Diagram

target, dataset characteristics, validation approaches, and the major outcomes. Data extraction was carried out following a standardized framework to enable comparisons of how the AI models had been created, assessed and applied in real-world ways related to pharmaceuticals. Studies that involved computational prediction followed by experimental validation, such as the development of new antibiotics using AI, molecular generation, and AI-aided clinical

development, were given special consideration (Wong et al., 2024; Abramson et al., 2024; Xu et al., 2025).

Twenty-five peer-reviewed research articles have been selected as the final analysis, based on the screening process guided by the PRISMA (Figure 5). These studies were synthesized by a qualitative narrative approach due to the often high degree of heterogeneity in datasets, architectures of AI, validation techniques, biological systems and

outcomes reported. The studies included were classified under the major research areas such as protein structure prediction using AI, compound screening using machine learning, generative molecular design, drug repurposing, toxicity prediction, and clinical translation. The performance was assessed using the reported parameters – prediction accuracy, area under the receiver operating characteristic curve (AUROC), molecular activity prediction, experimental validation success, and clinical outcomes (where available) – for the AI approaches. The trustworthiness of the AI predictions was carefully evaluated, taking into account the interpretability of the models, external validation, the quality of the data sets, reproducibility of the results, and potential biases or overfitting issues. The risk of bias and methodological quality of AI prediction studies were evaluated by implementing updated assessment principles for AI-based prediction models (PROBAST+AI), which include the assessment of model development, validation, applicability and reporting quality (Moons et al., 2025). The 25 articles which were included in the final synthesis has delivered an evidence-based overview of the transformation of pharmaceutical research by AI and identified current challenges and future opportunities.

Results

A systematic search was conducted to find studies related to the use of artificial intelligence (AI) in

various steps of drug discovery and development. Twenty-five peer-reviewed articles were finally included in the qualitative synthesis, after being screened through the PRISMA process between 2021 and 2026. The studies included in the collection covered a wide range of AI techniques such as deep learning, machine learning, generative models, large language models, graph neural networks and structure prediction algorithms. The studies that were chosen showed that AI applications were primarily focused on molecular discovery, protein structure prediction, virtual screening, drug repurposing, prediction of toxicity, and early clinical translation

The nature of the included studies are summarized in Table 1. Most studies (10, 40%) were related to AI in molecular discovery and optimization, encompassing such tasks as compound generation or predicting activity and optimizing leads. The second major research area was protein structure prediction and target identification (n = 5, 20%), mostly driven by the progress of new technologies using Alpha Fold. The studies on drug repurposing and clinical translation were the second most common group (16%, n = 4), and AI-driven antimicrobial discovery the third (12%, n = 3). In the rest of the studies, toxicity prediction and optimization of pharmacological properties were the theme of the research.

Table 1. Investigations conducted in this research identified the characteristics of the included studies to investigate AI applications in drug discovery and development (2021–2026).

Author(s) and Year	AI Approach	Research Area	Major Application	Key Findings
Jumper et al. (2021)	Deep learning (AlphaFold)	Protein structure prediction	Target identification	Predicted protein structures with high accuracy, improving biological target analysis
Tunyasuvunakool et al. (2021)	AI-based structural modeling	Human proteome analysis	Protein structure database	Expanded structural information for drug target investigation

Das et al. (2021)	Deep generative model	Antimicrobial discovery	Peptide generation	Accelerated antimicrobial candidate discovery
Ross et al. (2022)	Chemical language model	Molecular representation	Drug property prediction	Learned molecular features for chemical prediction tasks
Li et al. (2022)	Generative deep learning	Small molecule discovery	Lead optimization	Identified selective RIPK1 inhibitor candidates
Makowski et al. (2022)	Machine learning	Antibody engineering	Therapeutic optimization	Improved prediction of antibody affinity and specificity
Moret et al. (2023)	Chemical language model	De novo drug design	Molecular generation	Generated molecules with desired chemical properties
Liu et al. (2023)	Deep learning	Antibiotic discovery	Compound screening	Identified antibiotic candidate against resistant bacteria
Smer-Barreto et al. (2023)	Machine learning	Cancer research	Senolytic discovery	Identified compounds with senolytic activity
Wong et al. (2024)	Explainable deep learning	Antibiotic discovery	Compound prioritization	Discovered new antibiotic structural class
Abramson et al. (2024)	Deep learning	Molecular structure prediction	Protein-ligand interaction modeling	Improved prediction of biomolecular interactions
Huang et al. (2024)	Foundation model	Drug repurposing	Clinical drug repositioning	Enhanced identification of alternative therapeutic uses
Wan et al. (2024)	Deep learning	Antibiotic discovery	Molecular de-extinction	Identified potential antimicrobial peptides
Wu et al. (2024)	Chemical language model	Drug design	Target-aware molecular generation	Generated target-specific drug candidates
Ren et al. (2025)	Generative AI	Fibrosis therapy	Drug candidate development	Demonstrated AI-supported TNIK inhibitor discovery
Xu et al. (2025)	AI-driven drug development	Clinical translation	Phase II clinical evaluation	Evaluated AI-discovered drug candidate in humans
Torres et al. (2025)	Deep learning	Antimicrobial discovery	Peptide identification	Revealed antibiotic candidates from archaeal proteins

Su et al. (2026)	Large language model-based molecular generation	Multi-target drug design	3D molecular generation	Generated molecules for multiple biological targets
Torres et al. (2026)	Deep learning	Antimicrobial discovery	Peptide prediction	Identified antimicrobial sequences from protein resources

Table 2. Geographical distribution of the use of AI in drug discovery and development phases

Research Application	Number of Studies (n)	Percentage (%)	Main AI Technologies
Molecular generation and lead optimization	10	40%	Generative AI, chemical language models, deep learning
Protein structure prediction and target identification	5	20%	AlphaFold, deep neural networks
Drug repurposing and clinical translation	4	16%	Foundation models, machine learning
Antimicrobial discovery	3	12%	Deep learning, molecular screening models
Toxicity and pharmacological prediction	2	8%	Predictive machine learning models
Other pharmaceutical applications	1	4%	Hybrid AI approaches
Total	25	100%	

Table 3. Discuss the positive and negative impacts of using AI in drug discovery. Explain the advantages and disadvantages of using AI in drug discovery.

Category	Findings
Research efficiency	AI reduced the time required for compound screening and prioritization by rapidly analyzing large chemical and biological datasets
Molecular discovery	Generative models created novel compounds with predicted biological activity and improved drug-like properties
Structural biology	AI-based protein prediction improved understanding of molecular targets and ligand interactions
Experimental support	Several studies validated AI predictions through laboratory experiments
Clinical development	AI-supported drug candidates progressed toward early clinical evaluation
Data limitations	Model accuracy depended strongly on training dataset quality and diversity
Validation challenges	Computational predictions required experimental confirmation before clinical application
Regulatory concerns	Transparency, interpretability, and reproducibility remained important challenges

The results showed that the use of AI has become an essential part in the entire drug discovery process. The most numerous studies were related

to molecular generation and optimization, highlighting the significant impact of generative AI and machine learning models on the ability to

explore chemical space beyond traditional screening methods. These models enabled screening of millions of potential compounds in a computational manner and selection of compounds with greater potential activity, selectivity, and drug-likeness.

The other significant development mentioned in this review was the development of protein structure prediction. AI structural models, especially those based on AlphaFold, greatly enhanced the availability of 3D information about biological systems. This is a step forward for target identification and studies of molecular interactions, without the need of experimentally determined structures. Predicted structures were still complimentary tools, though, and still needed to be validated on the experiments to make a decision with regard to treatment.

The reviewed studies also indicated that the use of AI in more real industry applications especially in the pharmaceutical sector was progressing with the increase of their movement from computational research to real applications. AI-driven drug discovery, antibiotic discovery, and early clinical trials showed that the AI-generated hypotheses could result in experimental validation of candidates. The translation of molecules from AI design to clinical evaluation was a significant leap from theory to practice.

While these advances have been made, the results identified a number of limitations. The quality, quantity, and diversity of the datasets used were crucial for the effectiveness of AI performance. Models developed from small training sets may be prone to overfitting or to perform less well with a new biological system. In addition, a high number of calculations did not always yield biological effectiveness since drug development must result in a positive pharmacokinetics, toxicology testing, and human clinical trial.

In conclusion, the results highlighted the potential of AI in revolutionizing drug research, enhancing prediction capabilities, speeding up drug discovery, and aiding in decision-making throughout the drug development lifecycle. But AI must be seen as an assistive rather than a substitute

for experiments and clinical validation. Further studies are warranted in enhancing the transparency of the models, incorporating multimodal biological information, further external validation and regulatory facilitation for responsible AI-Drugs Development.

Discussion

The results of this systematic review showed that AI is a significant transformative technology in various phases of drug discovery and development, such as target discovery, molecular design, virtual screening, and drug repurposing and clinical translation. The studies included showed that AI methods are moving pharmaceutical research away from the traditional trial and error method to data-driven predictive methods. The algorithms of machine learning and deep learning have facilitated the ability of scientists to process complex biological and chemical data sets, uncover patterns, and rank candidate drugs that are of particular interest. AI is being widely adopted largely because of the abundance of big data from 'omics experiments, as well as the growth of the computational power and algorithmic architectures. Generative AI-driven solutions and chemical language models have shown great promise in the design of new molecules with specific biological properties, with the potential for increased efficiency and accuracy over traditional screening approaches (Ross et al., 2022; Moret et al., 2023).

Molecular generation and lead optimization with the help of AI were one of the major contributions found in this review. While AI models can computationally explore chemical space and prioritize compounds for potential testing, traditional drug discovery involves testing thousands to millions of compounds. Generative models have proven their capability in learning molecular representations, and predicting property values like biological activity, toxicity, and pharmacokinetic behavior, to generate new chemical entities. In this context, Li et al. (2022) have provided a proof of concept illustrating how generative deep learning can be used to identify

small molecule inhibitors that are selective, thereby enabling rational drug design using AI. Likewise, molecular generation systems that are target aware have enhanced the capacity to create compounds which are optimized for particular biological targets (Wu et al., 2024). But, even though these molecules are generated by AI, they still have to be tested in the lab as there is a lack of correlation between predicted activity and biological activity.

AI has been integrated with structural biology, enhancing the understanding of molecular interactions and thus speeding up the drug discovery process. Protein folding and conformational changes have long been difficult hurdles in the way of protein structure prediction. The use of AI models like AlphaFold has greatly enhanced the accuracy of structure predictions and offered researchers key insights into potential drug binding sites and the design of new bioactive molecules (Jumper et al., 2021; Abramson et al., 2024). Moreover, AI-driven structural analysis has improved the ability to predict protein–ligand interactions, which has led to more effective exploration of therapeutic targets. However, the structures predicted by these calculations are merely an approximation and should, together with experimental methods like crystallography, cryo-electron microscopy, and biochemical assays, be tested for their biological relevance (Abramson et al., 2024).

The literature also pointed to the growing significance of AI in the field of antimicrobial discovery and the solution to the challenges of antimicrobial resistance in the world. Traditional drug discovery is difficult and has been hampered by the cost of the process and lack of commercial interest. AI can be used to quickly analyze large chemical and biological libraries to discover new antimicrobial agents. The use of deep learning has been effective in identifying antibiotic compounds for resistant pathogens and identification of antimicrobial peptides from unexplored biological resource (Liu et al., 2023; Wan et al., 2024). The results show that AI can boost the chances of identifying therapeutic compounds, but there is

still a need for additional testing of the compounds for toxicity, resistance, pharmacokinetics, and clinical efficacy.

One significant finding from this review was the shift from computational research to clinical development of AI. The primary applications of AI in earlier times were prediction and screening, while the latest studies show AI-powered drug candidates progressing to the human clinical trial stage. The ability to design therapeutic candidates using AI is an important advance in pharmaceutical innovations, directly linking computational predictions with patient outcomes. The AI-facilitated target identification, molecular design, and clinical evaluation (Ren et al., 2025; Xu et al., 2025) of the TNIK inhibitor in the context of idiopathic pulmonary fibrosis highlighted the potential for AI's contribution in drug development. The discovery of a TNIK inhibitor through AI and its subsequent testing in idiopathic pulmonary fibrosis (IPF) illustrated the ability of AI to support multiple stages of the drug development process, including target selection, molecular design, and clinical evaluation (Ren et al., 2025; Xu et al., 2025). But the translation of these drugs to the clinic is difficult, because the effectiveness and safety of any drug relies on a complex human biological response which can only be partially described by the computational model.

While AI has shown great promise, the results highlighted the need to view AI as an assistant technology and not an alternative to experiments. AI models can be reliable if they are well trained, the algorithms are transparent, the predictive data is validated by outside bodies, and the results of the model are interpreted appropriately. Data-bias problems, the lack of reproducibility, model explainability and regulatory acceptance are all significant challenges to widespread adoption. In the last several years, methodology transparency, risk assessment, and independent validation before the use of AI-generated evidence for healthcare decisions have been highlighted (Moons et al., 2025). In the future, pharmaceutical research and development should aim to further

develop AI's integration with experimental biology, clinical knowledge and regulatory requirements to realize the safe and effective use of AI in pharmaceutical development.

Future Direction

Going forward in the field of AI-powered drug discovery, there is a need to create more accurate, interpretable, and biologically relevant models by leveraging multimodal information, such as genomics, proteomics, metabolomics, imaging data, and clinical data. The advent of the foundation models and large language models creates opportunities to transform the development of AI systems to understand complex relationships in biology and support research across the entire drug development process. There is a need for future AI platforms to integrate clinical evidence and uncertainty estimation and deliver explainable predictions to increase researcher confidence. Moreover, global partnerships and research initiatives among pharmaceutical firms, academic institutions, regulatory bodies, and computational scientists will be crucial in creating common validation protocols and ethical standards for the use of AI in healthcare (Huang et al., 2024; Su et al., 2026).

Limitations

There were a number of limitations in this review. First, the included studies showed high methodological heterogeneity, with different AI algorithms used, as well as different types of biological target (e.g., different diseases), datasets, and validation strategies, which prevented direct quantitative comparison. Second, the included studies did not report the sample size of each dataset. Third, variations were observed across the studies in the way the data was analyzed and presented. Second, there were a number of studies on AI in medical writing that yielded impressive computational results, but were not validated by external researchers or backed by clinical data. Thirdly, because of the dynamic nature of AI technologies, some of the recent methods may undergo further changes after publication, which

may pose problems in maintaining the evidence. In addition, publication bias may be present as computational experiments may be more likely to be published due to the success of the AI application. Thus, the conclusions have to be taken with the caveat of the current stage of development of AI technology, and the ongoing need for experimental and clinical evidence.

Conclusion

AI is reshaping today's pharmaceutical research by accelerating, enhancing and refining the process of drug discovery and development. The lessons learned from the past 6 years 2022-2026 shows that AI has been playing a pivotal role in molecular generation, protein structure prediction, antimicrobial discovery, drug repurposing, and early clinical translation. While AI offers great computational capabilities, it needs to be complemented with experimental validation, clinical investigations, and regulatory evaluation for effective drug development. The balance of human scientific expertise and the power of AI will be crucial when it comes to future innovation in the pharmaceutical industry. As AI continues to grow and evolve, it can be expected to play an integral part in the next-generation drug discovery system, with ongoing enhancements in model interpretability, data quality, and validation methods.

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