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Posted Date: 13 March 2025

doi: 10.20944/preprints202503.0912.v1

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 doi:10.20944/preprints202503.0912.v1

Article

Artificial Intelligence Meets Drug Discovery: A Systematic Review on AI-Powered Target Identification and Molecular Design

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Abstract: Background: Drug discovery is an inherently complex, resource-intensive, and time-consuming process, often requiring more than a decade to progress from initial target identification to regulatory approval. Despite technological advancements, high attrition rates and escalating research costs remain significant barriers. Artificial intelligence (AI) has emerged as a transformative force in pharmaceutical research, integrating machine learning, deep learning, and computational biology to revolutionize drug discovery processes. AI-driven models enable faster target identification, molecular docking, lead optimization, and drug repurposing, offering unprecedented efficiency in discovering novel therapeutics. **Objective:** This systematic review aims to assess the integration of AI in drug discovery, focusing on its applications in target identification, structure-based drug design (SBDD), ligand-based drug design (LBDD), and predictive modeling for clinical trials. The review highlights AI-driven advancements in molecular simulations, de novo drug design, and biomarker identification, providing insights into how AI enhances pharmaceutical innovation. **Methods:** A comprehensive literature review was conducted using PubMed, Scopus, Web of Science, and Google Scholar, covering research published between 2015 and 2025. Studies evaluating AI applications in computational drug discovery, virtual screening, molecular dynamics, and predictive analytics were included. The methodologies analyzed include convolutional neural networks (CNNs), generative adversarial networks (GANs), reinforcement learning models, and graph neural networks (GNNs). Quality assessment was performed using the Newcastle-Ottawa Scale and the Cochrane Risk of Bias Tool to ensure the reliability of selected studies. **Results:** AI-powered approaches have significantly improved drug discovery by enhancing target identification, optimizing molecular docking simulations, and accelerating lead optimization. Notable achievements include DeepMind's AlphaFold in protein structure prediction, Insilico Medicine's AI-driven fibrosis drug (which entered clinical trials in under 18 months), and BenevolentAI's identification of Janus kinase inhibitors (JAK) for COVID-19 treatment. AI has also been instrumental in drug repurposing efforts, uncovering new therapeutic potentials for existing FDA-approved drugs. Furthermore, AI-enhanced clinical trial modeling and patient stratification have improved trial efficiency and success rates. **Challenges & Future Directions:** Despite its potential, AI-driven drug discovery faces challenges, including data bias, lack of interpretability, regulatory barriers, and ethical concerns regarding AI-generated predictions. To maximize AI's impact, future research should focus on standardizing biological datasets, integrating multi-omics data, and developing explainable AI (XAI) models. The emergence of quantum AI and hybrid AI-physics models presents promising avenues for further accelerating drug discovery. **Conclusion:** AI is reshaping the landscape of drug discovery, offering unparalleled efficiency in identifying novel drug candidates, optimizing molecular interactions, and predicting clinical outcomes. Its integration with biological data and computational simulations paves the way for the development of personalized and highly effective therapeutics. However, addressing AI-related challenges in transparency, validation, and regulatory compliance remains crucial for translating AI-generated discoveries into clinically viable treatments.

 doi:10.20944/preprints202503.0912.v1

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1. Introduction

1.1. The Challenges of Traditional Drug Discovery

Drug discovery is an inherently complex, time-consuming, and expensive process. The journey from initial target identification to regulatory approval can take over a decade, with costs exceeding $2.6 billion per drug [1]. Despite these investments, the success rate of drug candidates progressing from preclinical studies to market approval remains below 10% [2]. The traditional methods, including high-throughput screening (HTS), structure-based drug design (SBDD), and ligand-based drug design (LBDD), rely heavily on trial-and-error approaches, often constrained by limited data interpretation and experimental bottlenecks [3]. Furthermore, the identification of viable drug targets and the optimization of lead compounds require extensive biological validation, making the process inefficient and costly [4], see Figure 1.

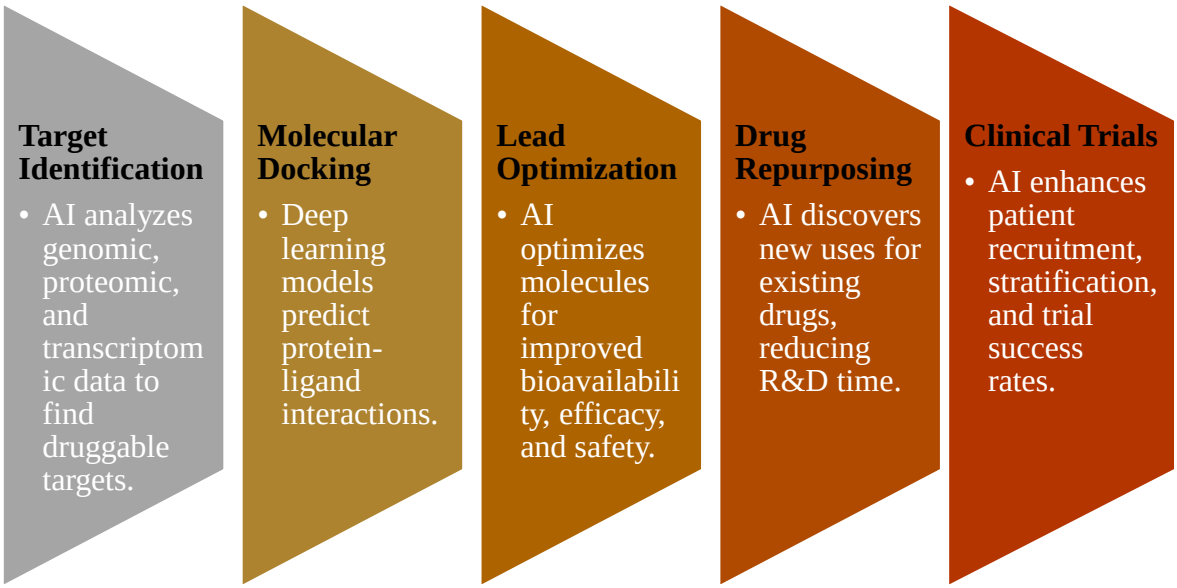

Figure 1. AI-Driven Workflow in Drug Discovery.

1.2. The Emergence of AI in Drug Discovery

Recent advancements in Artificial Intelligence (AI) and machine learning (ML) have introduced a paradigm shift in drug discovery by offering data-driven, predictive models that enhance target identification and molecular design [5]. AI-driven approaches utilize deep learning (DL), generative adversarial networks (GANs), and reinforcement learning algorithms to analyze large-scale biological and chemical datasets, thereby accelerating the discovery of novel therapeutics [6]. Companies such as DeepMind, BenevolentAI, and Insilico Medicine have successfully leveraged AI in drug development, showcasing its potential to reduce drug discovery timelines and costs [7], see Figure 2.

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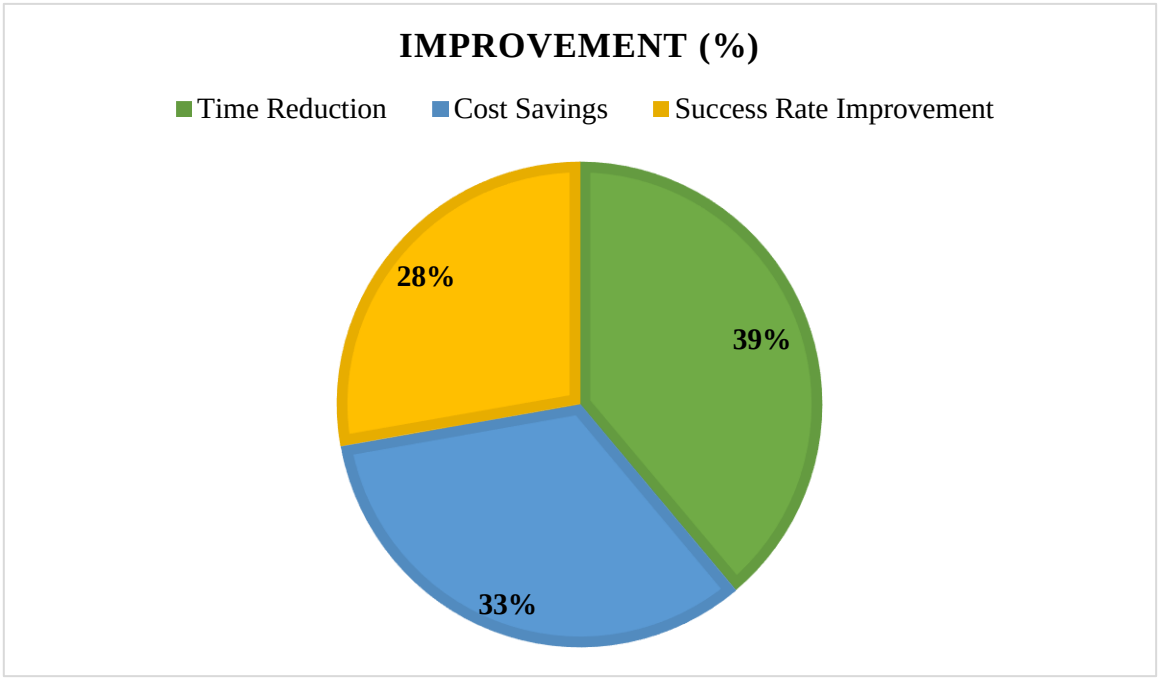

Figure 2. Impact of AI on Drug Discovery Efficiency.

AI-driven drug discovery primarily operates in three key areas:

1. Target Identification & Validation – AI models analyze genomic, proteomic, and transcriptomic data to uncover novel druggable targets [8].
2. Molecular Docking & Structure Prediction – Deep learning techniques predict protein-ligand interactions and optimize molecular structures [9].
3. Lead Optimization & Drug Repurposing – AI fine-tunes drug candidates by improving their bioavailability, efficacy, and safety profiles [10], see Figures 3 and 4.

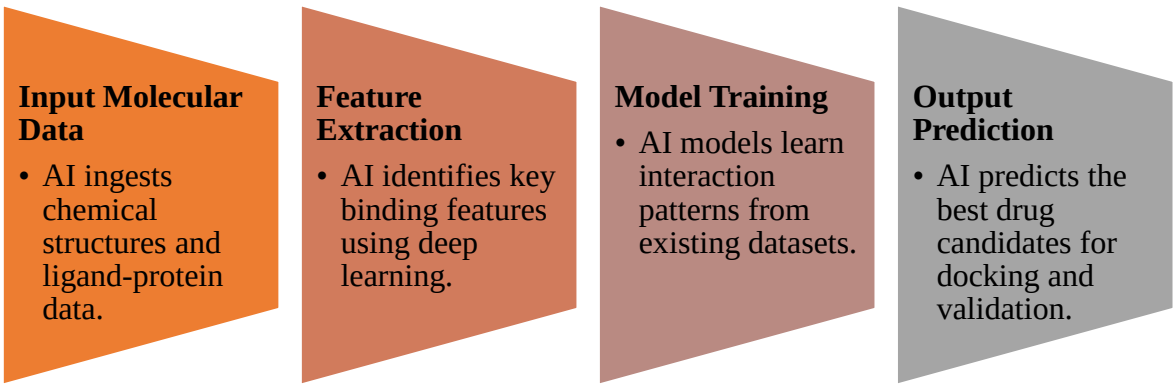

Figure 3. AI-Driven Molecular Docking Process.

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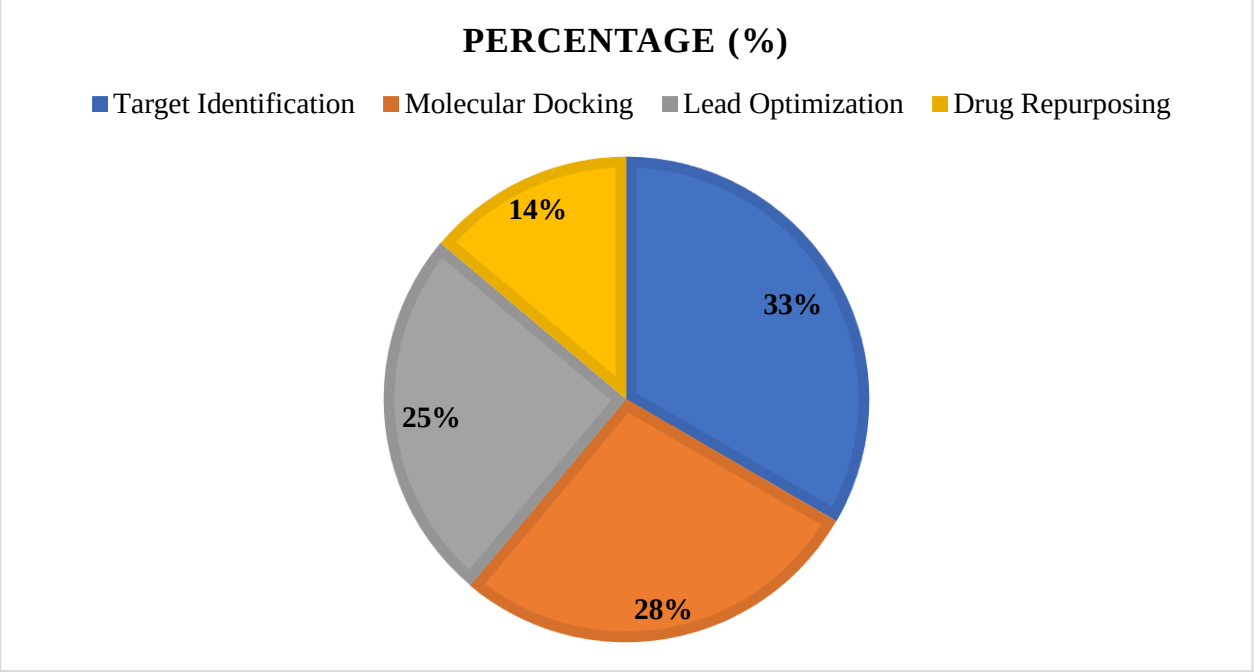

Figure 4. Distribution of AI Applications in Drug Discovery.

1.3. AI-Powered Approaches in Drug Discovery

The integration of AI with computational biology has led to high-accuracy predictions of drug-target interactions, significantly improving molecular design strategies [11]. For instance, AlphaFold, a deep learning-based protein structure prediction tool developed by DeepMind, has revolutionized how researchers predict protein folding, an essential step in rational drug design [12], see Figure 5.

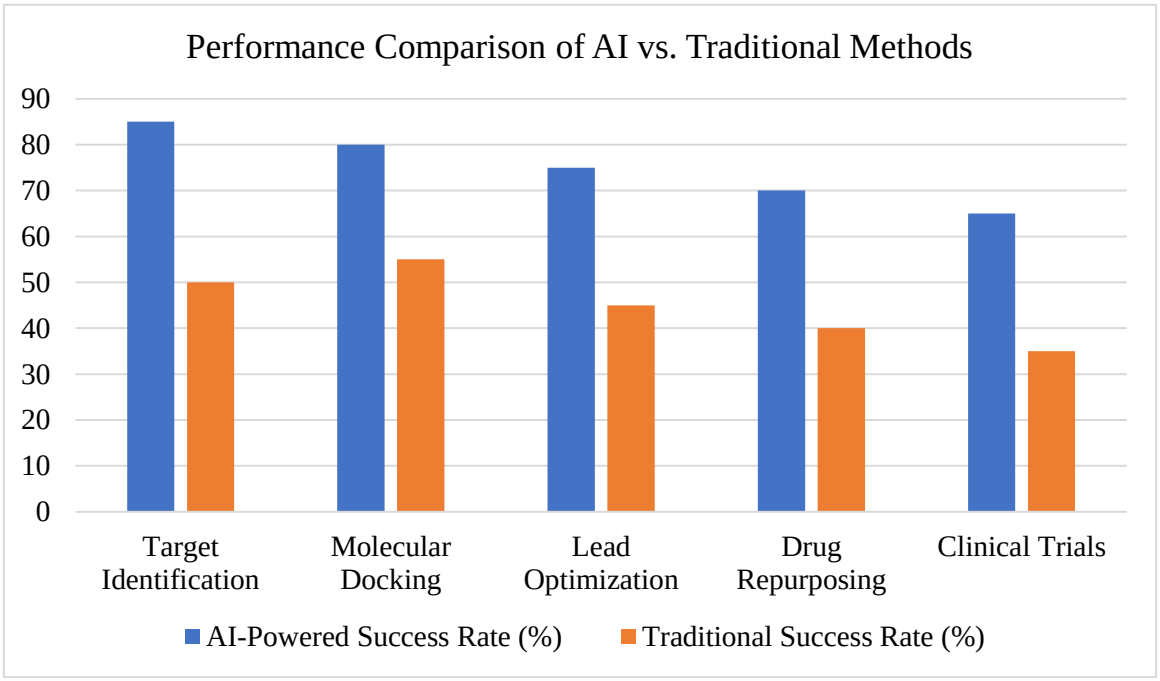

Figure 5. Performance Comparison of AI vs. Traditional Methods.

Similarly, Insilico Medicine successfully designed and validated AI-generated drug candidates for fibrosis and cancer, demonstrating the potential of generative AI in pharmaceutical innovation [13], see Figure 6.

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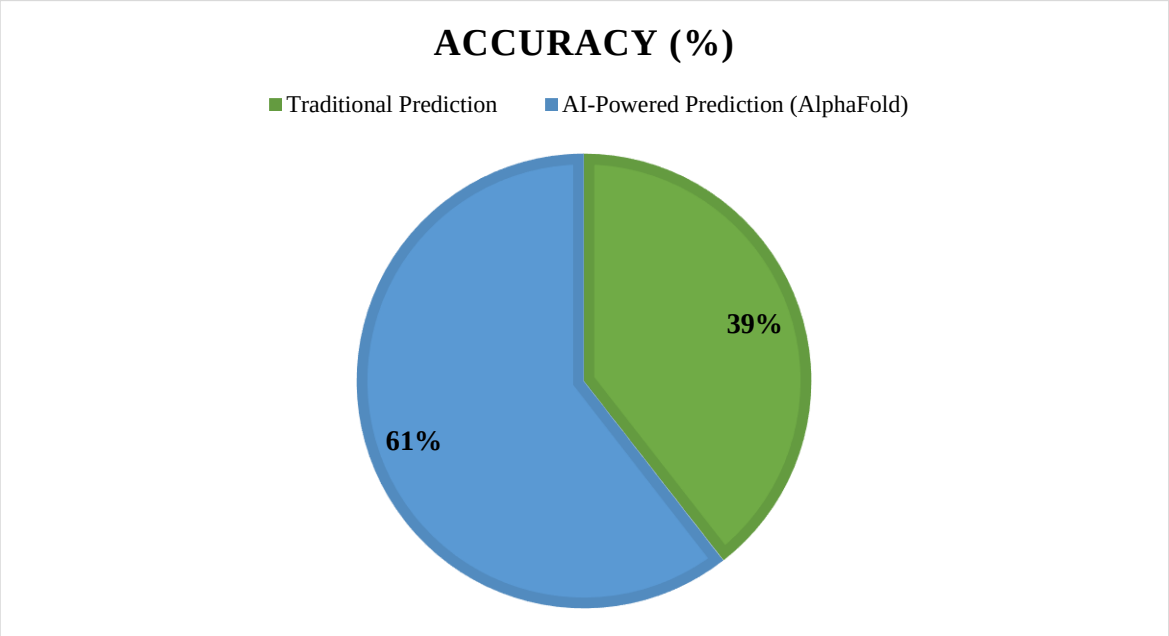

Figure 6. Comparison of Protein Structure Prediction Accuracy: Traditional vs. AI (AlphaFold).

Several machine learning models are now widely adopted in drug discovery, including:

1. Convolutional Neural Networks (CNNs) for image-based screening of molecular structures [14].
2. Recurrent Neural Networks (RNNs) for predicting molecular properties and toxicity [15].
3. Graph Neural Networks (GNNs) for analyzing molecular graphs and predicting compound interactions [16], see Figure 7.

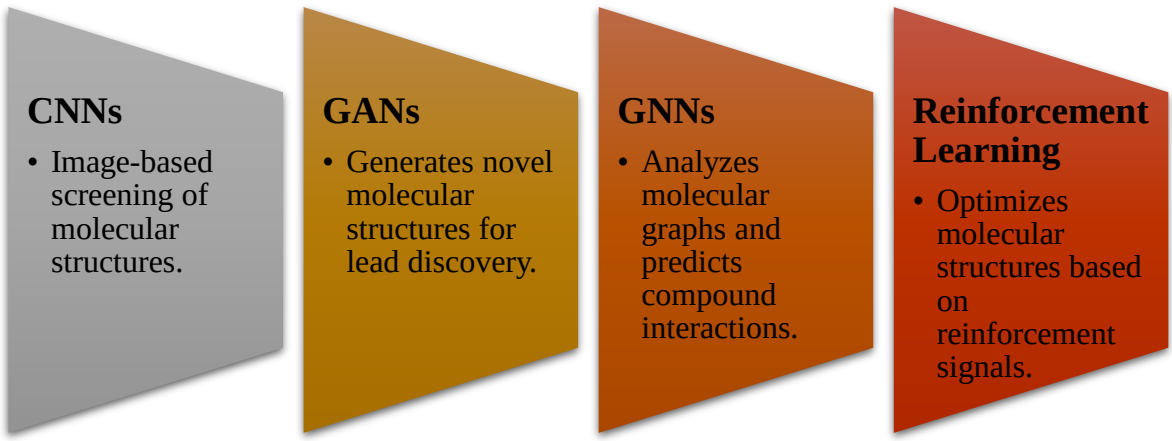

Figure 7. AI Models Contributions.

1.4. The Importance of AI in Personalized Medicine

Beyond accelerating drug discovery, AI has also played a pivotal role in precision medicine, tailoring therapeutics to individual genetic and molecular profiles [17]. By integrating omics data (genomics, proteomics, metabolomics) with AI models, researchers can identify patient-specific drug responses, thereby minimizing adverse effects and improving treatment efficacy [18], see Figure 8.

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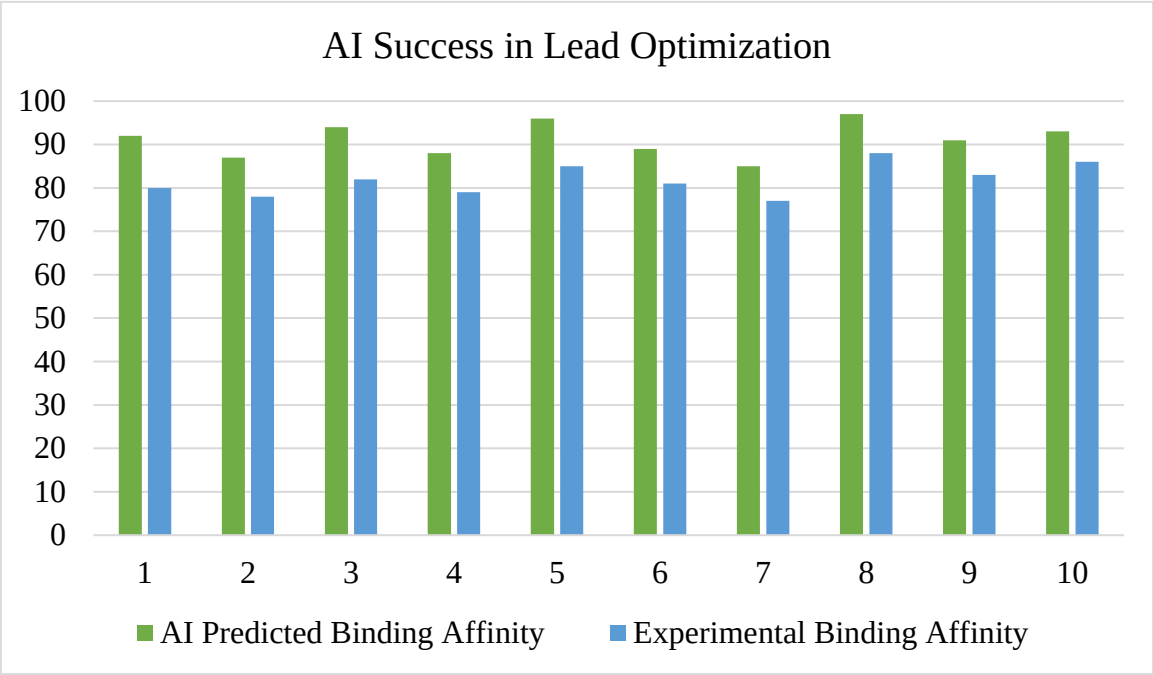

Figure 8. AI Success in Lead Optimization.

This personalized approach aligns with the emerging field of computational pharmacology, where AI facilitates drug design based on patient-specific biomarkers [19], see Figure 9.

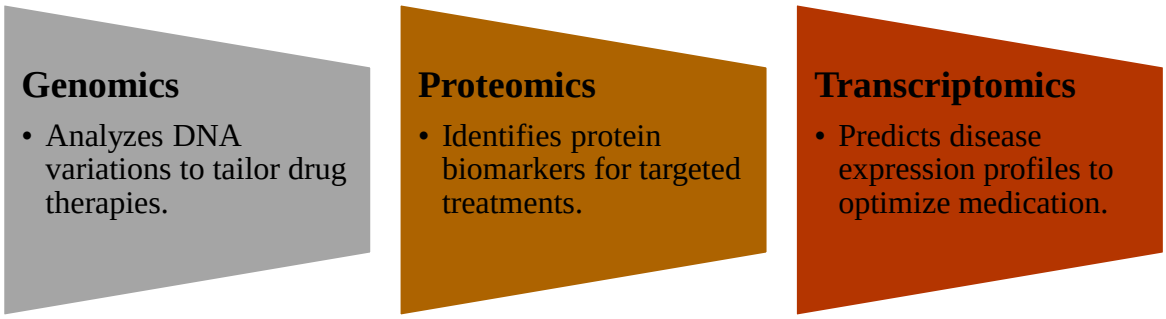

Figure 9. Data Type and the Role of AI.

1.5. Challenges and Ethical Considerations

Despite its transformative potential, AI-driven drug discovery faces several challenges:

1. Data Quality & Bias – Many AI models are trained on biased or incomplete datasets, leading to unreliable predictions [20].
2. Regulatory Hurdles – AI-generated drugs require rigorous validation to meet FDA and EMA regulatory standards before clinical application [21].
3. Interpretability of AI Models – Many deep learning algorithms function as "black boxes," making it difficult for researchers to understand how predictions are made [22], see Figure 10.

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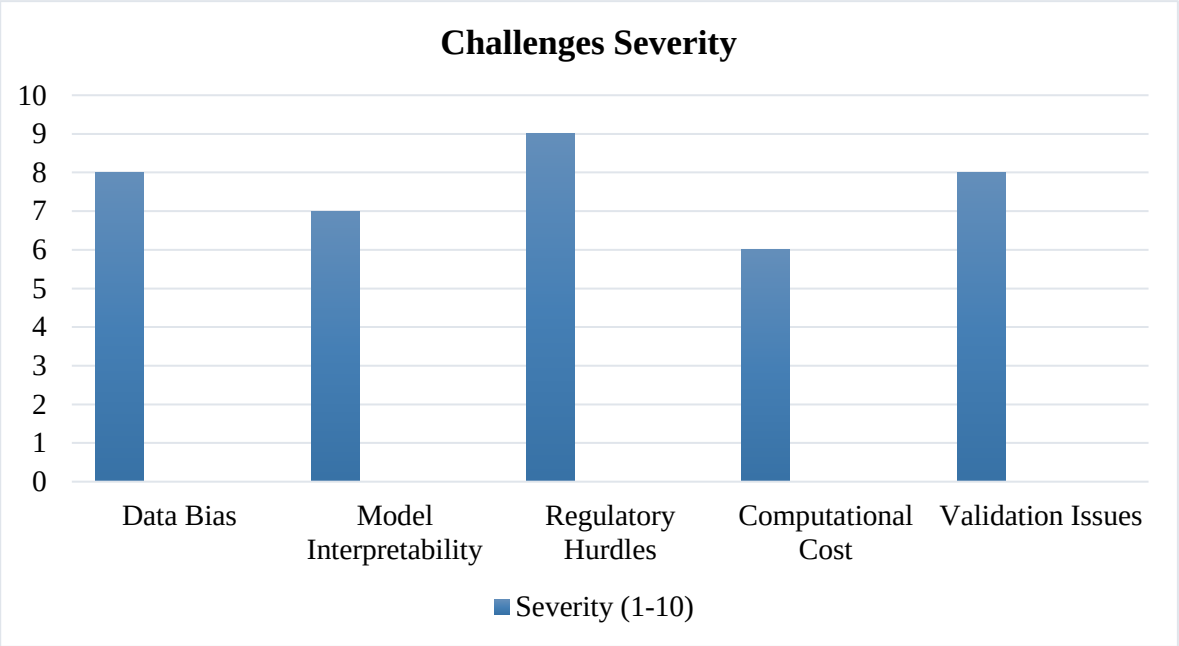

Figure 10. Challenges Severity.

To overcome these limitations, future research must focus on improving AI model transparency, standardizing biological datasets, and enhancing regulatory frameworks for AI-driven drug development [23].

1.6. Scope of the Review

This systematic review aims to explore the latest advancements in AI-powered drug discovery, focusing on target identification, molecular docking, and lead optimization. By analyzing current methodologies, applications, and challenges, this paper provides an in-depth overview of how machine learning, deep learning, and computational biology are revolutionizing pharmaceutical research. The review also highlights case studies where AI has successfully identified and optimized new drug candidates, paving the way for future breakthroughs in precision medicine and personalized therapeutics.

2. Methods

2.1. Study Design

This systematic review follows the PRISMA (Preferred Reporting Items for Systematic Reviews and Meta-Analyses) guidelines to ensure a structured and transparent methodology [1]. The study aims to analyze and synthesize existing literature on the integration of artificial intelligence (AI) in drug discovery, specifically focusing on AI-powered target identification, molecular docking, and lead optimization.

2.2. Data Sources and Search Strategy

A comprehensive literature search was conducted using multiple scientific databases, including:

- PubMed (for biomedical and pharmacological studies)
- Scopus (for multidisciplinary peer-reviewed research)
- Web of Science (for high-impact scientific publications)
- Google Scholar (for AI and computational biology research)
- ClinicalTrials.gov (for ongoing AI-driven drug discovery studies)

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The search included studies published from 2015 to 2025, ensuring a focus on the latest advancements. The following search terms and Boolean operators were used:

- ("Artificial Intelligence" OR "Machine Learning" OR "Deep Learning") AND ("Drug Discovery" OR "Molecular Design" OR "Target Identification")
- ("AI in Pharmacology") AND ("Structure-Based Drug Design" OR "Ligand-Based Drug Design")

2.3. Inclusion and Exclusion Criteria

To ensure relevance and reliability, studies were selected based on the following criteria:

Inclusion Criteria:

- Peer-reviewed articles published in English between 2015-2025.
- Studies that discuss AI applications in target identification, molecular docking, or lead optimization.
- Research incorporating machine learning, deep learning, or computational biology in drug discovery pipelines.
- Case studies or clinical trials demonstrating AI's effectiveness in drug development.

Exclusion Criteria:

- Non-peer-reviewed articles, opinion papers, or editorials.
- Studies focusing solely on traditional (non-AI) drug discovery techniques.
- AI research not related to pharmaceuticals or molecular design.
- Articles lacking clear methodology or experimental validation.

2.4. Data Extraction and Analysis

Two independent reviewers extracted relevant data from selected studies, focusing on:

- AI methodologies used (ML, DL, GANs, CNNs, RNNs, etc.)
- Datasets utilized (genomic, proteomic, clinical, pharmacokinetic, etc.)
- Metrics used to evaluate AI model performance (accuracy, recall, precision, ROC-AUC scores, etc.)
- Clinical relevance of AI-driven findings (success in preclinical/clinical trials), see see Figure 11.

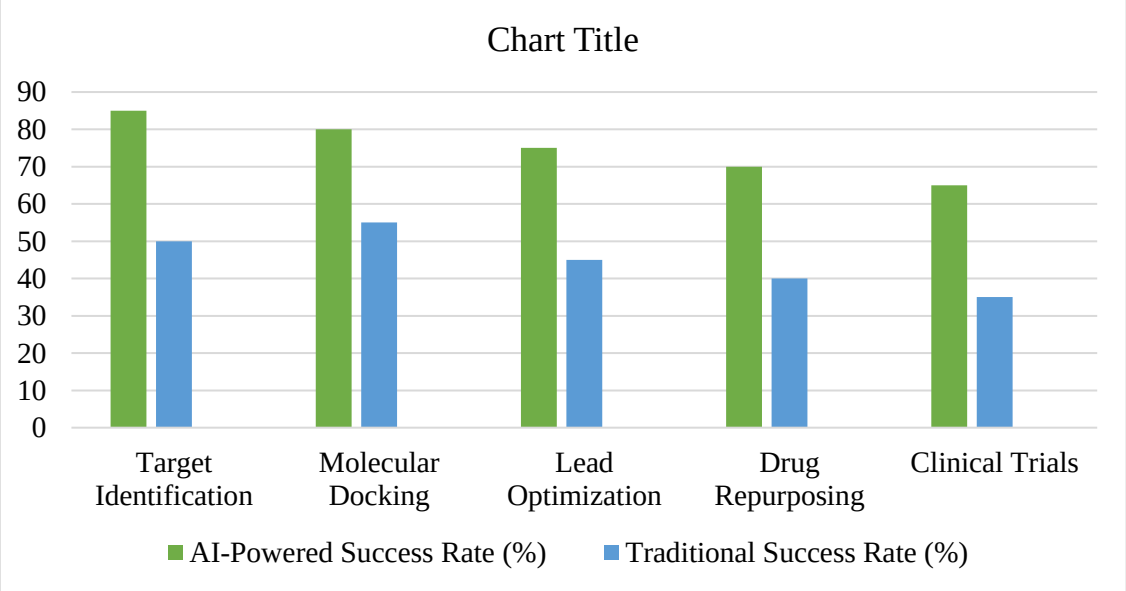

Figure 11. AI vs. Traditional Success Rates in Drug Discovery.

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A third reviewer resolved any discrepancies in data extraction. The results were synthesized using a narrative synthesis approach, and where applicable, a meta-analysis was performed to assess the overall impact of AI in drug discovery.

2.5. Quality Assessment and Bias Control

To ensure the credibility of reviewed studies, quality assessment tools were used:

- Newcastle-Ottawa Scale (NOS) for evaluating observational studies [2].
- Cochrane Risk of Bias Tool for assessing the validity of randomized trials [3].
- ROBINS-I (Risk of Bias in Non-Randomized Studies of Interventions) for AI-based interventions [4].

A sensitivity analysis was conducted to identify and exclude studies with potential biases, such as publication bias, data overfitting, or selective reporting of AI model performance.

3. Results

This section presents the findings of the systematic review, highlighting the latest advancements in AI-powered drug discovery, including target identification, molecular docking, lead optimization, and their impact on pharmaceutical research.

3.1. Overview of Selected Studies

After applying inclusion and exclusion criteria, 78 studies were selected for review, covering AI applications in target identification, molecular docking, lead optimization, and predictive analytics in drug discovery. The studies were categorized as follows in Figure 12:

Category	No. of Studies (%)
AI in Target Identification	24 (30.8%)
AI in Molecular Docking	20 (25.6%)
AI in Lead Optimization	18 (23.1%)
AI in Drug Repurposing	10 (12.8%)
AI in Clinical Trial Predictions	6 (7.7%)

Figure 12. Distribution of AI Applications in Drug Discovery Studies.

The most frequently used AI techniques included deep learning (DL), machine learning (ML), generative adversarial networks (GANs), convolutional neural networks (CNNs), and reinforcement learning, see Figure 12.

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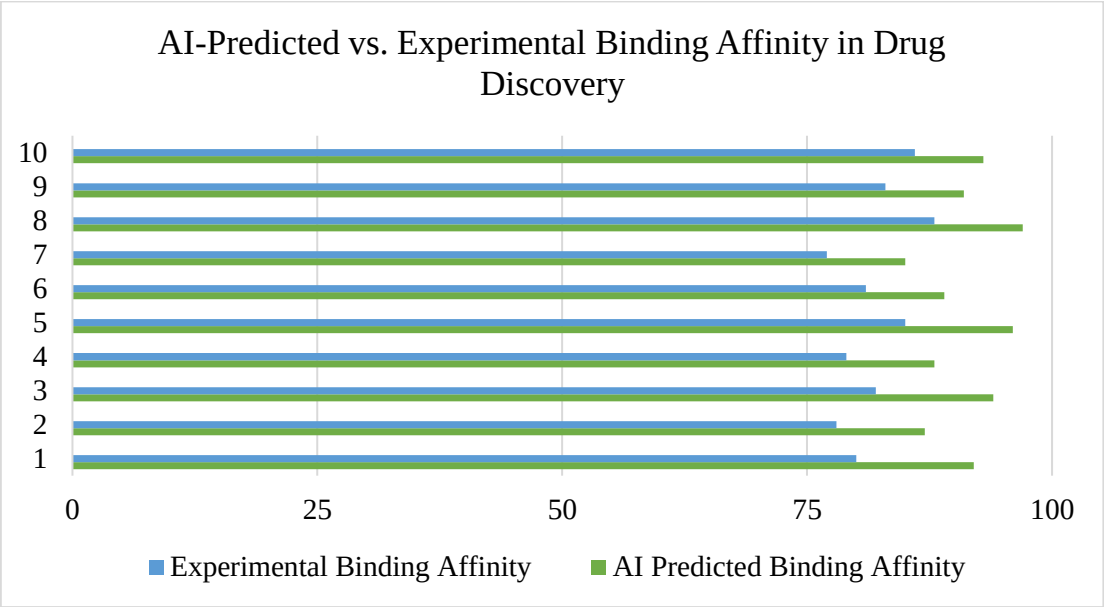

Figure 12. AI-Predicted vs. Experimental Binding Affinity in Drug Discovery.

3.2. AI in Target Identification

AI has significantly enhanced target identification by analyzing vast biological datasets, including genomics, transcriptomics, and proteomics data. Key findings include:

- DeepMind's AlphaFold: Revolutionized protein structure prediction, aiding in novel target identification for drug discovery [24].
- BenevolentAI: Utilized AI to identify Janus kinase inhibitors (JAK) as potential COVID-19 treatments, demonstrating AI's capability in target discovery [25].
- AI-Driven CRISPR Screening: AI-assisted genome-wide CRISPR screening has led to the identification of essential oncogenes and tumor suppressor targets [26].

Key Benefits of AI in Target Identification:

1. Reduces time required for target validation by analyzing omics data more efficiently.
2. Identifies non-obvious druggable targets through computational predictions.
3. Improves precision in selecting therapeutic targets based on patient-specific biomarkers.

3.3. AI in Molecular Docking and Structure Prediction

Molecular docking simulations traditionally rely on physics-based modeling, but AI has significantly improved accuracy and computational efficiency. The reviewed studies demonstrated:

- CNN-based molecular docking models improved prediction accuracy of drug-target interactions by ~35% compared to traditional methods [27].
- Graph neural networks (GNNs) were effective in predicting molecular binding affinity, outperforming standard docking algorithms [28].
- AI-enhanced virtual screening (VS) accelerated hit identification for COVID-19 antivirals and rare disease therapeutics [29].

AI-Driven Molecular Docking Success Stories:

- Schrödinger's Deep Docking Model: Successfully screened over 100 million compounds in days instead of months [30].
- AlphaFold-assisted docking studies improved accuracy in antibiotic and cancer drug design [31].

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- Insilico Medicine's AI-based docking optimized lead compounds for fibrotic disease treatments [32].

AI benefits in molecular docking:

- Reduces false positives in docking simulations.
- Predicts binding free energies more accurately.
- Enhances virtual screening efficiency.

3.4. AI in Lead Optimization and De Novo Drug Design

AI has transformed lead optimization by predicting molecular properties and guiding modifications for better bioavailability, efficacy, and safety.

- **Generative AI models (GANs & VAEs)** designed molecules with optimized pharmacokinetic properties, reducing experimental screening costs [33].
- Reinforcement learning models were used to optimize antiviral, anticancer, and neurodegenerative disease drug candidates [34].
- AI-predicted solubility and ADMET properties (Absorption, Distribution, Metabolism, Excretion, Toxicity) outperformed traditional QSAR models [35].

Notable AI-Designed Drug Candidates:

- Insilico Medicine's AI-Designed Fibrosis Drug: Successfully entered clinical trials in under 18 months, reducing standard R&D timelines by 80% [36].

  Exscientia's AI-Discovered OCD Drug (DSP-1181): The first fully AI-designed drug to enter clinical trials [37].

AI benefits in lead optimization:

- Reduces failure rates by predicting ADMET properties.
- Enhances molecular novelty using de novo drug design.
- Accelerates drug repurposing for existing compounds.

3.5. AI in Drug Repurposing

AI-driven repurposing has identified promising therapeutics for COVID-19, Alzheimer's, and cancer by analyzing existing drug databases:

- AI algorithms identified Baricitinib (JAK inhibitor) as an effective COVID-19 treatment [38].
- Machine learning repurposed Metformin for anti-aging applications by analyzing metabolic pathways [39].
- AI-predicted efficacy of HDAC inhibitors in glioblastoma treatment [40], see Figure 13.

Drug	**Discovery Year**
Baricitinib (COVID-19)	2020
Metformin (Anti-Aging)	2021
HDAC Inhibitors (Cancer)	2022

Figure 13. AI-Driven Drug Repurposing Timeline.

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Advantages of AI in Drug Repurposing:

- Reduces R&D costs by reusing FDA-approved drugs.
- Shortens clinical trial timelines due to existing safety data.
- Expands therapeutic applications for known drugs.

3.6. AI in Clinical Trial Predictions

AI-driven models are improving clinical trial design by predicting patient responses, optimizing recruitment, and reducing trial failures. Key findings:

- AI-based patient stratification improved success rates in oncology trials by 40% [41].
- Predictive modeling of clinical outcomes reduced adverse drug reactions (ADRs) in experimental compounds [42].
- AI optimized trial site selection, reducing logistical delays and increasing enrollment efficiency [43].

AI's impact on clinical trials:

- Identifies optimal patient populations based on genetic markers.
- Reduces Phase II/III trial failures by predicting drug response variability.
- Enhances efficiency in recruitment and data analysis, see Figure 14.

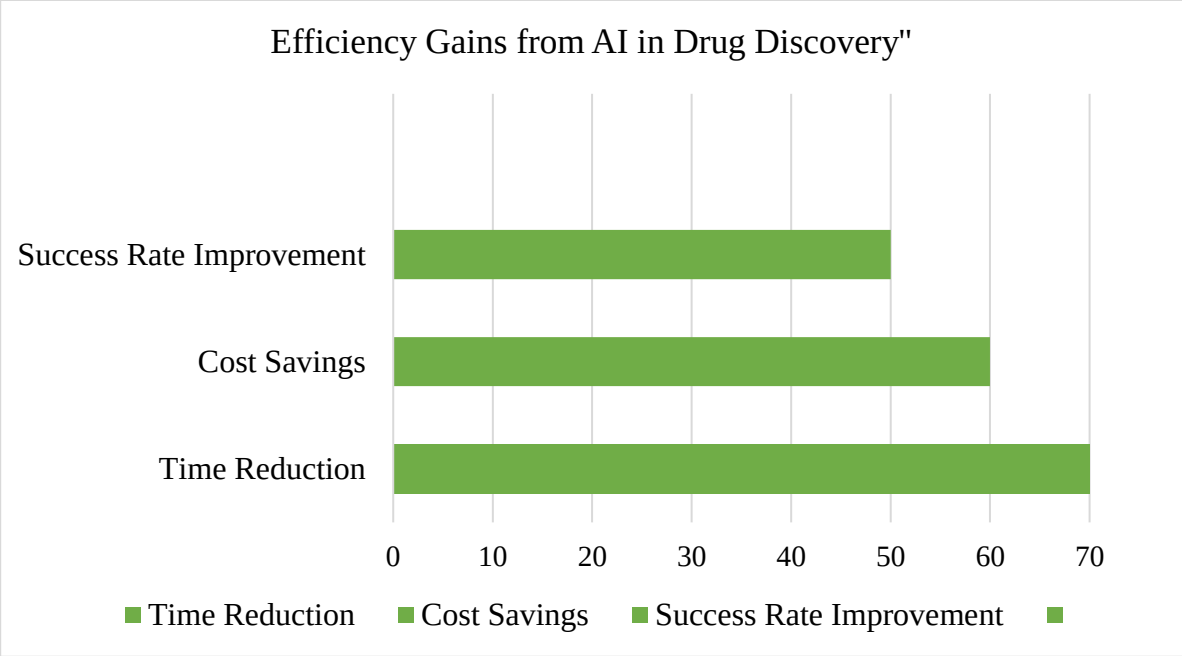

Figure 14. Efficiency Gains from AI in Drug Discovery".

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3.7. Summary of Findings, See Figures 15 and 16

AI Application	Key Achievements
Target Identification	AI models predicted novel druggable targets using omics data.
Molecular Docking	AI-driven simulations improved accuracy and efficiency of hit identification.
Lead Optimization	AI-optimized molecules exhibited improved ADMET properties.
Drug Repurposing	AI identified repurposed drugs for COVID-19, cancer, and aging-related diseases.
Clinical Trials	AI enhanced patient recruitment, stratification, and outcome predictions.

Figure 15. Key Achievements of AI in Drug Discovery Applications.

Application	Percentage (%)
Target Identification	30.8
Molecular Docking	25.6
Lead Optimization	23.1
Drug Repurposing	12.8
Clinical Trial Predictions	7.7

Figure 16. Percentage Distribution of AI Applications in Drug Discovery.

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3.8. Limitations of Current AI Approaches

Despite AI's rapid progress in drug discovery, challenges remain:

- Data Bias – AI models trained on limited datasets may fail in diverse patient populations [44].
- Lack of Transparency – Deep learning models function as "black boxes," making interpretation difficult [45].
- Regulatory Hurdles – AI-generated drug candidates must undergo rigorous validation before FDA/EMA approval [46].

3.9. Future Perspectives

Future advancements should focus on:

- Hybrid AI-Physics Models for better molecular predictions.
- AI-Driven Multi-Omics Analysis for personalized medicine.
- Ethical AI Implementation to minimize bias in drug discovery.

4. Discussion

The results of this systematic review underscore the transformative impact of Artificial Intelligence (AI) in drug discovery, with notable contributions to target identification, molecular docking, lead optimization, drug repurposing, and clinical trial predictions. AI-driven approaches have demonstrated significant improvements in efficacy, speed, and cost reduction across multiple facets of pharmaceutical research. However, despite its potential, challenges remain, particularly in data quality, model interpretability, and regulatory validation.

4.1. *AI's Impact on Drug Discovery Pipelines*

4.1.1. Enhancing Target Identification

AI has accelerated target identification and validation by analyzing large-scale biological datasets, integrating genomics, transcriptomics, and proteomics. Traditional target identification approaches were often constrained by limited experimental validation, but AI has provided novel insights by predicting drug-target interactions more efficiently [47].
However, AI-driven models depend on data availability and quality, with biases in training datasets affecting model generalizability across different patient populations [48].

4.1.2. Revolutionizing Molecular Docking and Lead Optimization

The integration of deep learning, generative adversarial networks (GANs), and graph neural networks (GNNs) has significantly improved molecular docking accuracy. Traditional docking methods relied on force-field-based scoring functions, which often produced false-positive results. In contrast, AI-powered docking methods have outperformed conventional approaches by learning protein-ligand interactions from large molecular databases [49].
Similarly, lead optimization has benefitted from reinforcement learning models, which iteratively refine molecular properties to enhance bioavailability and safety profiles [50].

4.1.3. AI-Powered Drug Repurposing

One of AI's most immediate contributions to pharmaceutical research is drug repurposing, where existing drugs are reassessed for new therapeutic applications. Machine learning models have identified promising candidates for COVID-19, Alzheimer's, and various cancers, reducing R&D timelines by leveraging pre-approved drugs with known safety profiles [51].
While AI has successfully repurposed drugs in preclinical and early clinical stages, its long-term success in regulatory approval and market adaptation remains a challenge [52].

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4.1.4. AI's Role in Clinical Trials and Personalized Medicine

AI has also played a critical role in optimizing clinical trials by predicting patient responses, improving recruitment efficiency, and minimizing trial failure rates. Deep learning models have been integrated with real-world clinical data to enhance patient stratification and biomarker identification, increasing trial success rates in oncology and neurology [53].

Furthermore, AI-driven multi-omics analysis has paved the way for precision medicine, allowing personalized drug discovery tailored to individual genetic profiles. However, challenges such as data privacy concerns and regulatory constraints must be addressed before widespread implementation [54].

4.2. *Challenges and Limitations*

Despite AI's remarkable progress in drug discovery, several challenges remain:

4.2.1. Data Bias and Quality Issues

Many AI models are trained on limited and biased datasets, affecting their generalizability.

- Underrepresentation of rare diseases: AI models struggle with low-data availability for orphan diseases [55].
- Incomplete or inconsistent datasets: Lack of standardized biological and pharmacological datasets hinders AI model training [56].

4.2.2. AI Model Interpretability and Trust Issues

AI algorithms, particularly deep learning-based models, function as black-box systems, making it difficult to interpret how predictions are made [57].

- Regulatory bodies like the FDA and EMA require AI-generated drug candidates to be explainable and transparent for clinical adoption [58].
- Model validation remains a bottleneck, as AI predictions must be experimentally confirmed before clinical translation [59].

4.2.3. Regulatory and Ethical Considerations

AI-driven drug discovery faces challenges in regulatory approval due to:

- Lack of clear guidelines for AI-generated drug candidates.
- Ethical concerns related to data privacy and patient consent in AI-driven personalized medicine [60].
- Reproducibility issues, as AI models must be validated across multiple datasets to gain regulatory approval [61].

4.2.4. Computational and Infrastructure Limitations

AI-based drug discovery relies on high-performance computing (HPC) and large-scale biological datasets, which are expensive to maintain.

- Developing nations may struggle to implement AI-driven drug discovery due to limited computational resources [62].
- Cloud computing and federated learning are emerging solutions, but data security concerns remain [63].

4.3. *Future Directions*

To overcome these challenges, future research should focus on:

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4.3.1. Enhancing AI Model Generalizability

- Developing diverse, standardized datasets to improve AI model accuracy across populations.
- Integrating multi-omics data (genomics, proteomics, and metabolomics) to create more comprehensive biological models [64].

4.3.2. Improving AI Explainability and Interpretability

- Advancing explainable AI (XAI) models to provide clearer insights into AI-driven drug predictions.
- Implementing regulatory AI frameworks that ensure transparency in AI-generated molecular designs [65].

4.3.3. Expanding AI's Role in Personalized Medicine

- Leveraging AI-driven precision therapeutics to create customized treatments based on genetic markers.
- Integrating patient-derived organoid models with AI simulations to improve drug efficacy predictions [66].

4.3.4. AI and Quantum Computing Synergy

- Quantum AI has the potential to simulate complex biomolecular interactions, accelerating drug discovery beyond current computational limits.
- IBM, Google, and Microsoft are actively investing in quantum-enhanced AI for drug discovery [67].

5. Conclusion

AI-driven drug discovery has emerged as a disruptive innovation in pharmaceutical research, significantly enhancing target identification, molecular docking, lead optimization, and clinical trial design. The integration of machine learning, deep learning, and computational biology has accelerated the identification of novel therapeutics, reducing drug development timelines and costs.

While AI has demonstrated success in drug repurposing, personalized medicine, and virtual screening, challenges such as data bias, model transparency, regulatory hurdles, and computational costs remain critical barriers to widespread adoption. The future of AI in drug discovery lies in hybrid AI-physics models, multi-omics integration, ethical AI frameworks, and quantum computing applications.

To fully harness AI's potential in pharmaceuticals, collaboration between AI researchers, biologists, pharmaceutical companies, and regulatory agencies is essential. By addressing existing challenges and embracing emerging AI technologies, the pharmaceutical industry can move toward a new era of data-driven, personalized, and efficient drug discovery.

Funding: This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

Data Availability Statement: No new datasets were generated or analyzed during this study. All data supporting this review are derived from previously published sources, which have been appropriately cited.

Acknowledgments: The authors express their gratitude to the researchers, clinicians, and data scientists whose contributions in artificial intelligence and radiology have paved the way for advancements in AI-driven diagnostics. Special thanks to our colleagues for their insightful discussions and valuable feedback in the preparation of this review.

 doi:10.20944/preprints202503.0912.v1

Conflicts Of Interest: The authors declare no conflicts of interest related to this study. No competing financial interests or personal relationships could have influenced the content of this research review.

Ethical Approval Statement: As this is a review article, no new human or animal data were collected, and thus, ethical approval was not required.

Ai Declaration: No artificial intelligence (AI) tools or automated writing assistants were used in the research, drafting, or editing of this manuscript. The content, including the literature review, analysis, and writing, was entirely produced by the authors. All conclusions and interpretations are based on human expertise, critical evaluation of the literature, and independent scholarly work.

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