SunText Review of Pharmaceutical Sciences
ISSN: 2766-5232
Open Access
Research Article
Volume 7:1

Computer-Aided Drug Design and Artificial Intelligence in Drug Discovery: Accelerating Pharmaceutical Innovation

Samantaray US[1,*] and Raj A[2]

[1]*Indian Institute of technology Patna, Bihar, India*
[2]*Dy Patil school of biotechnology and bioinformatics Navi Mumbai, India*

[*]**Corresponding author:** Samantaray US, Indian Institute of technology Patna, Bihar, India; E-mail: utkalendu_pa2501mbh457@iitp.ac.in

Received date: 04 June 2026; **Accepted date:** 11 June 2026; **Published date:** 21 June 2026

Citation: Samantaray US, Raj A (2026) Computer-Aided Drug Design and Artificial Intelligence in Drug Discovery: Accelerating Pharmaceutical Innovation. SunText Rev Pharm Sci 7(1): 140.

DOI: https://doi.org/10.51737/2766-5232.2026.040

Abstract

The pharmaceutical industry faces significant challenges in discovering and developing new therapeutic agents due to high costs, lengthy development timelines, and low success rates. Traditionally, bringing a new drug from laboratory research to market requires approximately 10–15 years and billions of dollars in investment. Recent advances in Computer-Aided Drug Design (CADD), Artificial Intelligence (AI), and Machine Learning (ML) have revolutionized the drug discovery process by enabling rapid target identification, virtual screening, lead optimization, and toxicity prediction. These technologies facilitate data-driven decision-making, improve efficiency, and reduce dependence on extensive laboratory experimentation. AI-powered drug discovery platforms have already demonstrated success in identifying novel drug candidates for cancer, fibrosis, infectious diseases, and rare disorders. Furthermore, regulatory authorities such as the U.S. Food and Drug Administration (FDA) are actively supporting the integration of AI-based methodologies into pharmaceutical research through various guidance frameworks and modernization initiatives. This review discusses the principles of CADD, the role of AI and ML in modern drug discovery, their impact on reducing development timelines, notable success stories, and the evolving regulatory landscape.

Key words: Computer-aided drug design; Artificial intelligence; Machine learning; Drug discovery; FDA; Virtual screening; Drug development

Introduction

Drug discovery is a complex and resource-intensive process involving target identification, hit discovery, lead optimization, preclinical studies, clinical trials, and regulatory approval. Despite technological advancements, the overall success rate of drug candidates remains low, with many compounds failing due to inadequate efficacy, toxicity, or poor pharmacokinetic properties. To address these challenges, computational approaches have become increasingly important in pharmaceutical research. Computer-Aided Drug Design (CADD) emerged as a powerful tool that enables researchers to model molecular interactions, predict biological activity, and optimize chemical structures before synthesis and experimental testing. In recent years, Artificial Intelligence (AI) and Machine Learning (ML) have further transformed the field by analyzing large biological datasets, predicting molecular behavior, and generating novel drug candidates. The integration of computational chemistry, bioinformatics, and AI is creating a new paradigm for drug discovery that emphasizes speed, efficiency, and precision.

Literature Review

The application of computational methods in drug discovery began with molecular modeling and structure-based design approaches in the late twentieth century. Advances in protein crystallography and molecular docking enabled scientists to visualize protein-ligand interactions and predict binding affinities. Structure-Activity Relationship (SAR) and Quantitative Structure-Activity Relationship (QSAR) studies became essential tools for understanding how molecular features influence biological activity. These approaches significantly improved the rational design of drug candidates. The emergence of high-throughput screening generated massive biological datasets that paved the way for machine learning applications. Researchers began utilizing algorithms such as Random Forests, Support Vector Machines, Neural Networks, and Deep Learning models to predict biological activity, toxicity, and pharmacokinetic properties. Recent studies have demonstrated that AI-based approaches can identify promising drug candidates with greater speed and accuracy than traditional screening methods. Deep learning models have shown remarkable success in protein structure prediction, molecular generation, and target identification, establishing AI as a transformative force in pharmaceutical research.

Computer-Aided Drug Design (CADD)

Computer-Aided Drug Design refers to the use of computational tools and algorithms to facilitate the discovery and optimization of therapeutic compounds.

Structure-based drug design (SBDD)

Structure-Based Drug Design relies on the three-dimensional structure of a biological target. Protein structures obtained through X-ray crystallography, Cryo-Electron Microscopy (Cryo-EM), or Nuclear Magnetic Resonance (NMR) spectroscopy are used to identify potential binding sites and design molecules that interact with them.
Common techniques include:

- Molecular Docking
- Molecular Dynamics Simulation
- Pharmacophore Modelling
- Binding Free Energy Calculations

These methods enable researchers to prioritize compounds with high binding affinity before experimental validation (Figure 1).

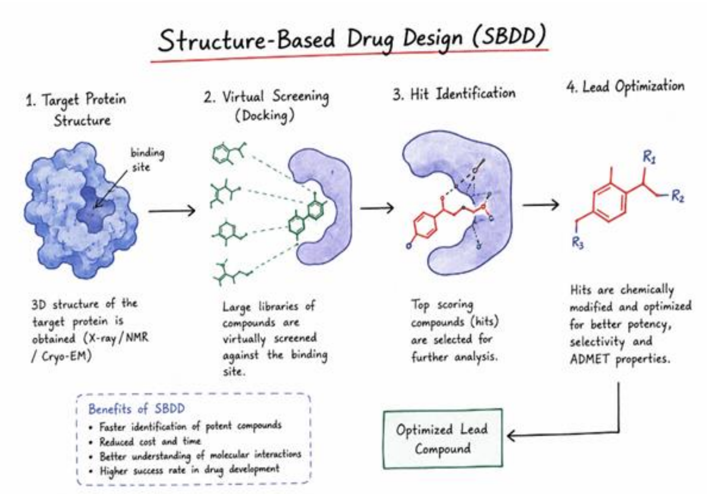

Figure 1: *Structure-Based Drug Design (SBDD).*

Ligand-based drug design (LBDD)

Ligand-Based Drug Design is applied when the target protein structure is unavailable. It relies on information obtained from known active compounds.
Techniques include:

- QSAR Modelling
- Pharmacophore Mapping
- Similarity Searching
- Machine Learning-Based Prediction

LBDD helps identify new molecules with biological properties similar to known therapeutics (Figure 2).

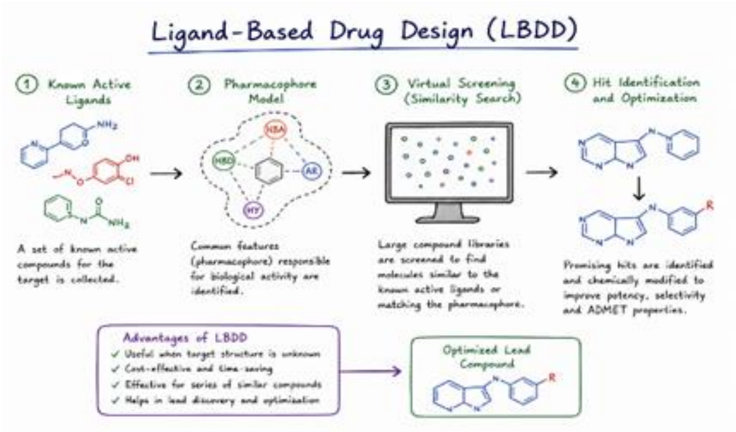

Figure 2: *Ligand-Based Drug Design (LBDD).*

Advantages of CADD

The major advantages include:

- Reduction in laboratory screening costs
- Faster identification of lead compounds
- Improved prediction of drug-likeness
- Enhanced optimization of pharmacokinetic properties
- Reduced attrition rates during development

Artificial Intelligence and Machine Learning in Drug Discovery

Artificial Intelligence refers to computer systems capable of performing tasks that traditionally require human intelligence. Machine Learning is a subset of AI that enables systems to learn patterns from data and improve predictive performance.

Applications of AI in drug discovery

Target Identification

AI algorithms analyze genomic, proteomic, transcriptomic, and clinical datasets to identify disease-associated targets.

Virtual Screening

Machine learning models rapidly evaluate millions of compounds and prioritize candidates with the highest probability of success.

Lead Optimization

AI predicts molecular properties such as potency, selectivity, solubility, and metabolic stability, enabling rapid optimization of lead compounds.

Toxicity Prediction

Predictive models identify potential toxic effects early in development, reducing costly late-stage failures.

Drug Repurposing

AI can identify new therapeutic applications for existing drugs by analyzing disease pathways and molecular interactions.

Generative AI in drug discovery

Generative AI represents one of the most significant recent advances in pharmaceutical research.
Techniques include:

- Variational Autoencoders (VAEs)
- Generative Adversarial Networks (GANs)
- Transformer Models
- Reinforcement Learning Algorithms

These models can design entirely new molecular structures optimized for specific biological targets and therapeutic properties.

Reduction in Drug Discovery Timeline

Traditional drug development requires approximately 10–15 years from initial discovery to market approval.
AI and ML technologies significantly accelerate early-stage drug discovery by automating data analysis and reducing experimental iterations (Table 1).

Table 1: *Reduction in Drug Discovery Timeline.*

Development Stage	Traditional Duration
Target Identification	1–2 Years
Hit Discovery	2–3 Years
Lead Optimization	1–2 Years
Preclinical Development	1–2 Years
Clinical Trials	6–8 Years
Total	10–15 Years

Major time-saving contributions include:

- Automated literature mining
- Rapid virtual screening
- Early toxicity prediction
- Computational lead optimization
- Faster biomarker identification

Several reports suggest that AI-assisted discovery platforms can reduce early discovery timelines from 4–6 years to less than 1–2 years, representing a substantial improvement in efficiency.

Real-World Success Stories

Insilico Medicine

Insilico Medicine utilized generative AI to identify novel therapeutic targets and design a candidate drug for idiopathic pulmonary fibrosis. The AI-driven discovery process progressed from target identification to preclinical candidate selection in less than 18 months, significantly faster than conventional approaches.

Exscientia

Exscientia developed AI-designed drug candidates that entered clinical trials within approximately one year of project initiation. Their platform integrates machine learning with medicinal chemistry to optimize compounds rapidly.

Benevolent AI and COVID-19

During the COVID-19 pandemic, Benevolent AI applied machine learning algorithms to identify Baricitinib as a potential therapeutic option. The prediction was later supported by clinical evidence and contributed to treatment strategies during the pandemic.

AlphaFold

Developed by DeepMind, AlphaFold transformed structural biology by accurately predicting protein structures from amino acid sequences. This breakthrough has accelerated target identification and structure-based drug design across numerous therapeutic areas.

FDA Perspective and Regulatory Prioritization

The U.S. Food and Drug Administration recognizes the growing importance of AI and computational modeling in pharmaceutical development.

FDA Initiatives Supporting AI

The FDA has introduced several initiatives to encourage innovation while maintaining safety and scientific integrity.
These initiatives focus on:

- Model-Informed Drug Development (MIDD)
- Computational Modeling and Simulation
- Digital Health Innovation
- Real-World Evidence Integration
- AI Governance Frameworks

Model-Informed Drug Development (MIDD)

MIDD incorporates mathematical modeling and simulation to support regulatory decision-making throughout drug development. Benefits include:

- Optimized clinical trial design
- Improved dose selection
- Reduced development costs
- Faster regulatory evaluation

FDA Expectations for AI Systems

The FDA emphasizes:

- Transparency
- Data Quality
- Reproducibility
- Explainability
- Validation and Verification
- Patient Safety

The agency encourages pharmaceutical sponsors to engage regulators early when AI tools are incorporated into development programs.

Future Regulatory Outlook

As AI technologies continue to evolve, regulatory agencies are expected to establish more comprehensive frameworks addressing:

- Generative AI applications
- Adaptive machine learning systems
- Validation standards
- Risk management strategies
- Ethical use of AI in healthcare

These developments indicate increasing regulatory acceptance of AI-assisted drug discovery methodologies [1-8].

Challenges and Limitations

Despite significant progress, several challenges remain.

Data Availability and Quality

Machine learning models require large, high-quality datasets. Incomplete or biased data may compromise predictive accuracy.

Model Interpretability

Many deep learning systems operate as "black boxes," making it difficult to explain predictions.

Biological Complexity

Human biological systems remain highly complex, and computational predictions must always be validated experimentally.

Regulatory Considerations

Standardized validation procedures for AI-based tools are still under development.

Ethical Concerns

Important considerations include:

- Data privacy
- Algorithmic bias
- Transparency
- Reproducibility

Addressing these issues is critical for broader adoption.

Conclusion

Computer-Aided Drug Design, Artificial Intelligence, and Machine Learning are fundamentally reshaping modern drug discovery. By enabling rapid target identification, virtual screening, lead optimization, and toxicity prediction, these technologies significantly reduce development timelines and improve efficiency. Successful examples from companies such as Insilico Medicine, Exscientia, and Benevolent AI demonstrate the practical impact of AI-driven approaches. Simultaneously, the FDA is actively supporting the integration of computational tools through Model-Informed Drug Development programs and emerging AI governance frameworks. As data availability, computational power, and algorithmic sophistication continue to improve, AI-enabled drug discovery is expected to become a cornerstone of future pharmaceutical innovation, ultimately accelerating the delivery of safer and more effective therapies to patients worldwide.

References

1. Paul D, Mytelka DS, Dunwiddie CT, Persinger CC, Munos BH, Lindborg SR, et al. How to improve R&D productivity: the pharmaceutical industry's grand challenge. Nature Reviews Drug Discovery. 2010; 203-214.
2. Jumper J, Evans R, Pritzel A, Green T, Figurnov M, Ronneberger O, et al. Highly accurate protein structure prediction with AlphaFold. Nature. 2021; 583-589.
3. Vamathevan J, Clark D, Czodrowski P, Dunham I, Ferran E, Lee G, et al. Applications of machine learning in drug discovery and development. Nature Rev Drug Discovery. 2019; 463-477.
4. Schneider G. Automating drug discovery. Nature Reviews Drug Discovery. 2017; 97-113.
5. FDA. Model-informed drug development (MIDD) Pilot Program Guidance.
6. Insilico medicine publications on AI-driven drug discovery.
7. Exscientia clinical development reports.
8. Benevolent AI COVID-19 drug repurposing studies.

Citation: Samantaray US, Raj A (2026) Computer-Aided Drug Design and Artificial Intelligence in Drug Discovery: Accelerating Pharmaceutical Innovation. SunText Rev Pharm Sci 7(1): 140.