International Journal of Pharmacy and Pharmaceutical Science 2025; 7(2): 366-372

International Journal of Pharmacy and Pharmaceutical Science

ISSN Print: 2664-7222
ISSN Online: 2664-7230
Impact Factor (RJIF): 8.25
IJPPS 2025; 7(2): 366-372
www.pharmacyjournal.org
Received: 02-08-2025
Accepted: 05-09-2025

Dr. ND Nizamuddin
Professor, Department of Pharmaceutical Chemistry, Dr K V Subba Reddy Institute of Pharmacy, Dupadu, Kurnool, Andhra Pradesh, India

Sravani Sugali
Student, Dr. K. V. Subba Reddy Institute of Pharmacy, Dupadu, Kurnool, Andhra Pradesh, India

Corresponding Author:
Dr. ND Nizamuddin
Professor, Department of Pharmaceutical Chemistry, Dr K V Subba Reddy Institute of Pharmacy, Dupadu, Kurnool, Andhra Pradesh, India

Artificial intelligence and Machinery Learning (ML) derived drug discovery good machine learning practice

ND Nizamuddin and Sravani Sugali

DOI: https://doi.org/10.33545/26647222.2025.v7.i2e.228

Abstract
It includes how Artificial intelligence (AI) and machine learning (ML) are transforming the pharmaceutical sector, especially in drug discovery and development. It provides a comprehensive review of recent advancements from 2019 to 2024 regarding AI-driven approaches, such as deep learning, generative adversarial networks, and data-driven methodologies, that accelerate and improve various stages of drug research. The document evaluates innovative model architectures, cloud-based implementations, and their roles in preclinical analysis, safety, hit/lead discovery, and target identification. It highlights the challenges in traditional drug discovery, including long timelines, high costs, and low success rates, and demonstrates how AI and ML address these by enhancing virtual screening, lead optimization, and target validation. Ultimately, the work underscores that robust AI integration can revolutionize pharmaceutical R&D, offering promising solutions to accelerate innovation and optimize patient outcomes.

Keywords: Machine learning, drug discovery**,** data quality, predictive toxicology, artificial intelligence, target identification

Introduction
The pharmaceutical industry's use of AI has changed dramatically in the last several years. Early AI applications in drug development, in the 1980s and 1990s, were restricted to simple computational models, mostly utilised for chemical structure prediction and molecular modelling. AI has been used by pharmaceutical corporations into many phases of drug research, from designing clinical trials to identifying targets. AI has emerged as a key instrument in recent years for improving clinical trials, speeding up drug discovery, and customising therapies, signalling a move towards more effective, data-driven pharmaceutical research and development [1, 2, 3] This has enabled AI to fuel drug repurposing by easing the identification of new therapeutic uses for existing pharmaceuticals and hastening their clinical translation from bench to bedside. This is especially significant for parasite diseases that impact developing countries, as well as orphan diseases [4, 5]
Continued collaboration between researchers, physicians, industry stakeholders, and regulatory agencies is critical to driving AI innovation in the pharmaceutical business. [6]

2. Literature Review
1. Dolores R Serrano *et.al* (2024) AI is transforming the pharmaceutical industry through advanced computational methods. It accelerates drug discovery, personalized medicine, and treatment optimization. Applications include target identification, excipient selection, and manufacturing processes. While enhancing efficiency and outcomes, AI also raises regulatory challenge

2. Gongxing Chen *et.al* (2024) Computational tools are transforming drug discovery by improving efficiency, lowering costs, and reducing risks in preclinical and clinical trials.

Machine learning, particularly deep learning, enhances virtual screening, molecular design, and complex synthesis. AI technologies play key roles in drug screening, molecular design, and addressing clinical trial challenges. Future directions focus on overcoming AI-related limitations to advance drug discovery and development

3. Scope and Boundaries

The latest developments in artificial intelligence and machine learning (AI/ML) as they relate to drug discovery from 2019 to 2024 are thoroughly examined in this review. The focus of the scope is on contemporary model architectures and cloud-based implementations that are especially pertinent to applications in the pharmaceutical sector.

3.1 AI in Drug Discovery

The process of identifying and developing novel pharmaceutical substances for commercial distribution is known as drug discovery. The average time to finish this multi-stage process is fifteen years. Pharmacovigilance will continue to be used to monitor the drug's safety throughout its distribution after it is put on the market (Figure 1)

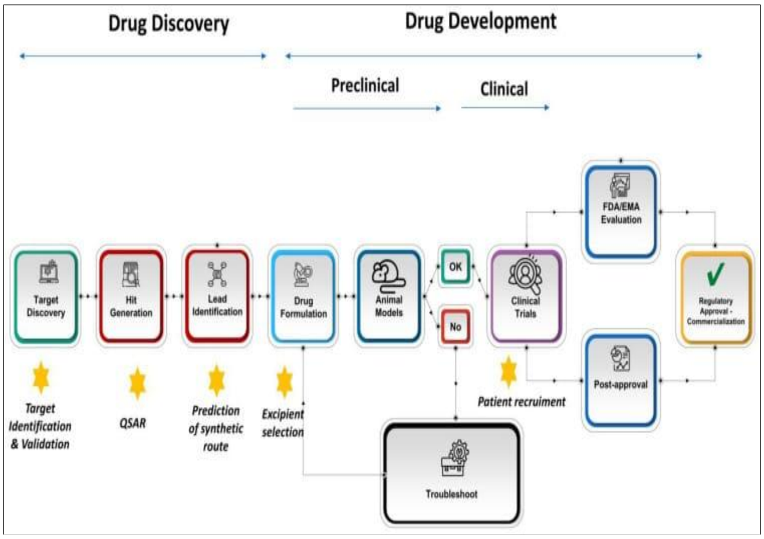

Fig 1: A schematic depicting the key phases of the drug development and discovery process. The steps of the pharmaceutical process where AI is crucial are represented by the star.

Furthermore, AI algorithms have played a critical role in the development of medicinal compounds with increased potency and selectivity. Using deep learning algorithms and generative adversarial networks (GANs), AI can design optimised chemical structures that target certain biological activities while satisfying specific pharmacological and safety characteristics [7]. In drug discovery, the generator can build novel chemical structures that imitate known drugs that have desirable features. During training, the generator continuously increases its ability to generate realistic samples, while the discriminator gains proficiency in spotting fakes. This adversarial process continues until the generator creates enough samples for the discriminator to no longer distinguish between bogus and real data [8].

In order to speed up the drug discovery process and lower the chance of clinical trial failure, a number of AI-powered drug discovery platforms, like Atomise [9, 10] and Benevolent AI [11], are prioritising specific drug targets with the highest likelihood of therapeutic success. This is revolutionising the way that new leads are currently found. These platforms analyse a variety of datasets, such as proteomic, genomic, and clinical data, using machine learning algorithms to find new therapeutic targets and forecast their draggability. [12]

Over the past ten years, AI-driven drug discovery has produced encouraging outcomes in a variety of therapeutic domains, including rare disorders, neuroscience, infectious diseases, and oncology. For instance, the Alpha Fold algorithm from DeepMind employs deep learning principles to predict protein structures with exceptional accuracy, providing important information about interactions between proteins and ligands [13]. Because of this, researchers have only been able to examine a small portion of these proteins, which has seriously hampered efforts to find new drugs and treat illnesses. Predicting the forces of attraction and repulsion that eventually determine a protein's three-dimensional structure is necessary to unravel its structure (14)

Even while AI-driven drug discovery has made great strides, there are still a number of issues that need to be addressed. AI models are complicated and challenging to comprehend due to their interpretability, particularly deep learning models. [15]

3.2 ML in Drug Discovery

Large-scale datasets of chemical compounds, biological targets, and molecular interactions are used by machine learning algorithms to quickly analyse intricate relationships and more accurately and efficiently identify prospective drug candidates. [16]

- **Virtual Screening**

The practice of computationally screening enormous compound libraries to find possible therapeutic candidates is known as virtual screening. In the early phases of drug discovery, it is a crucial step [17]

The primary benefit of machine learning-based virtual screening is its ability to extract intricate patterns and connections from enormous databases of biological targets and chemical substances. [18] In virtual screening, support vector machines (SVMs), random forests, and deep learning models are some of the most popular machine-learning techniques that have been effectively implemented.

- **Target Identification**

A crucial stage in the drug development process is identifying appropriate drug targets, which determines the molecular mechanisms and biological pathways that can be altered to provide therapeutic effects. Target identification is a critical function of machine learning algorithms. Through the examination of various genomic, proteomic, and clinical data sets, these algorithms find possible targets linked to disease and rank them for additional research. [19]

Machine learning algorithms can use dimensionality reduction techniques like principal component analysis (PCA) and t-distributed stochastic neighbour embedding (t-SNE) to uncover hidden relationships between biological entities and identify potential drug targets based on their expression patterns, functional annotations, and disease associations. [20]

Additionally, machine learning algorithms are able to combine data from multiple sources in order to rank potential drug targets according to their therapeutic relevance, safety profiles, and druggability. [21] In order to identify possible targets based on their transcriptional fingerprints and functional annotations, the connectivity map (CMap) also employs machine learning techniques to examine gene expression profiles from drug-treated cells. [22]

- **Lead optimization**

Lead optimisation uses iterative chemical alterations to enhance the potency, selectivity, and pharmacokinetic characteristics of possible therapeutic candidates after they have been identified. GANs and QSAR modelling are two machine learning techniques that have grown in prominence. This is why the DeepChem framework employs deep learning algorithms to accurately predict the biological activities of novel molecule analogues and to directly learn molecular representations from chemical structures [23]. By using molecular docking simulations, Schrödinger's Maestro platform prioritises lead candidates for additional optimisation and forecasts the binding affinities of novel compounds to target proteins. [24]

3.3 ML Algorithms in Drug Discovery

ML algorithms have made substantial advances in drug discovery. Pharmaceutical businesses have benefited substantially from the use of various machine learning algorithms in drug discovery. ML algorithms have been used to construct multiple models for predicting chemical, biological, and physical features of molecules in drug development. [25, 26, 27, 28] ML algorithms can be used at every stage of the drug-discovery process. to guarantee safety biomarkers, forecast drug-protein interactions, develop new uses for medications, and maximise molecular bioactivity, for instance, machine learning techniques have been applied. [29, 30, 31] ML techniques that have been extensively employed in drug discovery include support vector machines (SVM), random forest (RF), and naive Bayesian (NB), among others. [32]

3.4 Basic Steps in Machine learning

Prior to applying AI machine learning workflows to pharmaceutical industrial processes, it is essential to comprehend the fundamental procedures involved in creating precise and accurate AI machine learning workflows (Figure 1).

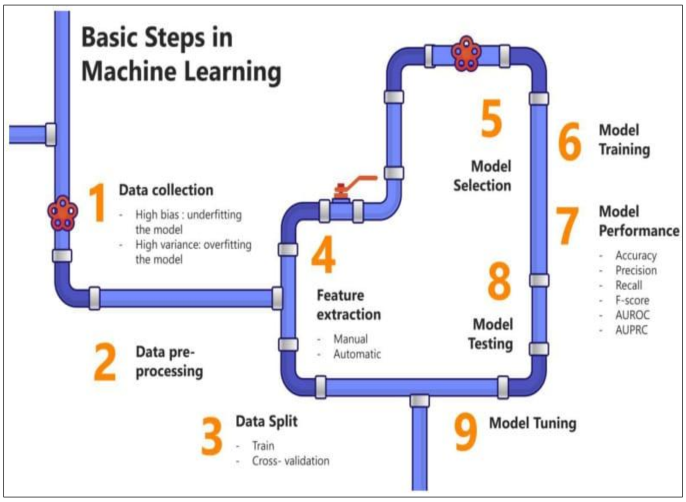

Fig 2: Basic steps in machine learning

4. The Drug Discovery Process

- **Over view of traditional drug discovery**

The goal is to understand the target's function in the onset of the disease and assess its importance for therapeutic intervention

a) **Optimisation**: After identifying possible lead compounds, the next step is optimisation. To improve the pharmacokinetic, efficacious, and selective properties of the leads, this involves changing their chemical structure

b) **Preclinical Studies:** To evaluate a lead molecule's pharmacokinetics, safety, and effectiveness after optimisation, preclinical research is conducted in animal models.

- **Challenges in Traditional Drug Discovery**

There are numerous important obstacles in the way of traditional drug discovery:

a) **Extended Timelines:** It may take up to ten years from target identification to market approval in the drug discovery process.

b) **Low Success Rates**: The majority of drug candidates fail to go past the preclinical or clinical phases, which suggests that drug research has a comparatively low success rate.

- **The Role of AI and ML in Drug Discovery:** The application of artificial intelligence (AI) and machine learning (ML) in drug discovery has revolutionised the pharmaceutical industry and offers promising solutions to the issues associated with traditional drug development processes. [33]

Finding Hits At this point, the goal is to find tiny molecules or biologics that can interact with the chosen targets. Traditional high-throughput screening methods take a lot of time and money. Improvement of Leads After hits are identified, these compounds need to be optimised to minimise toxicity and increase pharmacokinetic, selectivity, and efficacy. AI and machine learning models are used to forecast how modifications to the molecular structure would affect these characteristics. [34] Advancement In preclinical and clinical stages, AI and ML help forecast the toxicity, bioavailability, and adverse effects of drug candidates as well as optimise dosage schedules. [35]

4.1 AI and ML Techniques in Drug Discovery

- **Machine Learning Algorithms**

Medication development has been completely transformed by machine learning (ML) techniques, which allow for the study of enormous datasets in order to find novel compounds, forecast their biological action, and improve medication design.

a) **Supervised Learning:** One of the methods in drug discovery that is most frequently employed is supervised learning. It entails using a labelled dataset—where the target values are known—and input data (features) to train a model. Two well-liked methods in this area are supervector machines (SVM) and random forests (RF).

b) **Unsupervised Learning:** When there are no labelled outputs in the dataset, unsupervised learning techniques are used to find patterns or structures in the data. By using these methods, new chemotypes can be found and investigated further in the process of developing new drugs.[36, 37, 38, 39]

- **Data Source and Processing**

Large, high-quality datasets are crucial to the creation of machine learning (ML) and artificial intelligence (AI) models in the drug discovery process. Large-scale chemical and biological data are mostly provided by extensive databases such as PubChem, ChEMBL, and the Protein Data Bank (PDB) [39]. These varied datasets make it possible for AI models to produce insights at the chemistry-biology interface, which promotes creativity in drug discovery.

However, there are certain obstacles to overcome when using large datasets, especially when processing data. The initial significant challenge is data curation, which involves gathering pertinent, accurate, and comprehensive data from diverse sources. [41]

- **AI Driven Drug Design**

These technologies have revolutionized the process since the advent of artificial intelligence, increasing productivity and hastening the discovery of new drugs. Predicting possible drug candidates has become a popular use for generative models, such as variational autoencoders (VAEs), generative adversarial networks (GANs), and reinforcement learning (RL) methods.

4.2 Overview of AI in Drug Discovery and Development

'AI' refers to a broad set of technologies that enable machines to mimic human intellect, such as learning, reasoning, and decision-making [42]. ML, a subset of AI, allows systems to learn from data and improve their performance on certain tasks via experience, all without the need for explicit programming. DL is a subset of ML that uses Artificial Neural Networks (ANN) with numerous layers ("deep" networks) to detect complicated patterns and draw meaningful insights from data [43,44]

AI methods have clear benefits for drug discovery. Tasks like virtual screening and drug-target identification are carried out by machine learning techniques like support vector machines (SVMs) and random forests (45,46) (Fig. 1). New methods like GNN and Gen-AI can be used to provide enough unique and varied datasets for efficient model training.

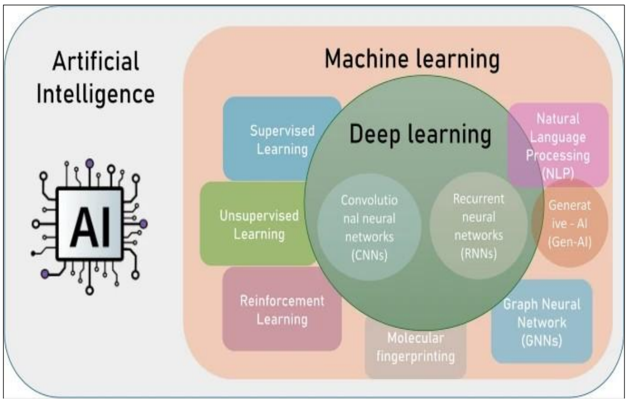

Fig 3: Overview of Artificial Intelligence: Machine Learning and Deep Learning Approaches

The main elements of artificial intelligence are summarised. Natural language processing, machine learning, deep learning, neural networks, molecular fingerprinting, graph neural networks, and generative artificial intelligence (AI) are among the fundamental elements of AI, as are their interactions in AI-driven systems.

5 Future Prospects

- **Emerging Trends in AI And Drug Discovery**

Recent technological advancements have sparked a revolution in drug research and development, with artificial intelligence (AI) at the forefront. One of the most intriguing concepts is the fusion of quantum computing and AI algorithms.

- **Collaborative Efforts**

To fully achieve AI's potential in drug research and development, cooperation between pharmaceutical companies, AI developers, academic institutions, and regulatory authorities is essential. Large datasets and in-depth domain expertise are two things pharmaceutical businesses offer that are crucial for AI algorithm training.

5.1 Challenges and Limitations

- **Data Quality and Availability**

The availability and quality of data have a significant impact on the effectiveness of AI models in drug research and discovery. There are several difficulties in this situation.

a) **Data Quality Issues:** The quality of the data used directly affects how effective AI models are. Incomplete, noisy, or inconsistent datasets are examples of low-quality data that can produce unreliable models and erroneous forecasts.

b) **Limited Data Availability:** Large-scale, high-quality datasets are frequently hard to get by because of acquisition costs or proprietary restrictions.

c) **Lack of Standardization:** The integration and comparison of datasets from many sources are made more difficult by the lack of uniform data formats and protocols.

d) **Bias and Representativeness:** Biased data may have been used to train AI models, which could result in models that do not generalize well across various populations or environments.

- **Model Interpretability**

Because many machine learning (ML) methods, such deep neural networks, are intrinsically opaque, interpreting AI models is a big difficulty, especially in the context of complicated domains like drug research and development. Although these models, also called "black boxes," can produce accurate forecasts, they reveal very little about the methodology used to generate them.

6. Results

- **Advanced technologies in drug discovery**

According to the results of our literature search, the pharmaceutical industry today uses a variety of technologies and methods to support drug manufacturing and development. The ADMET platform (Bayer, Leverkusen, Germany) is one of these technologies. Due to the cost barrier,A third innovative technology currently used in the pharmaceutical industry is 3D printing.

- **Machine Learning in drug discovery**

The use of machine learning is increasing in various avenues of the pharmaceutical industry, including drug discovery, enabling improvements in the industry as a whole. The achievements of machine learning are demonstrated by the expanding number of companies in which ML is key to their business structure.

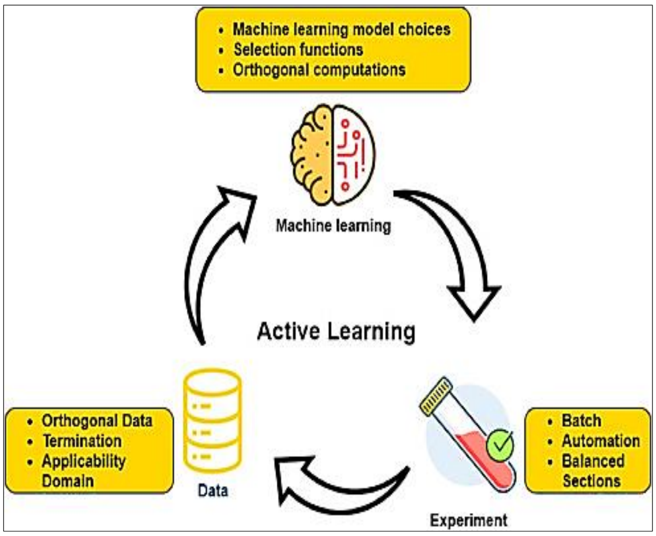

Fig 4: Machine learning in drug discovery

The aim was to determine a certain machine learning algorithm could be used as a substitute for animal testing to predict the bitterness of different molecules used in drugs. Overall, 80% of the identified bitter molecules matched those obtained from a brief access taste aversion (BATA) experiment, indicating that this study was successful.

- **Artificial intelligence in drug discovery:** Enhanced computational power and the development of innovative techniques in the field of AI could be used to reform drug discovery and development processes. In this section, the main uses of AI to improve the effectiveness of the drug discovery cycle are discussed.

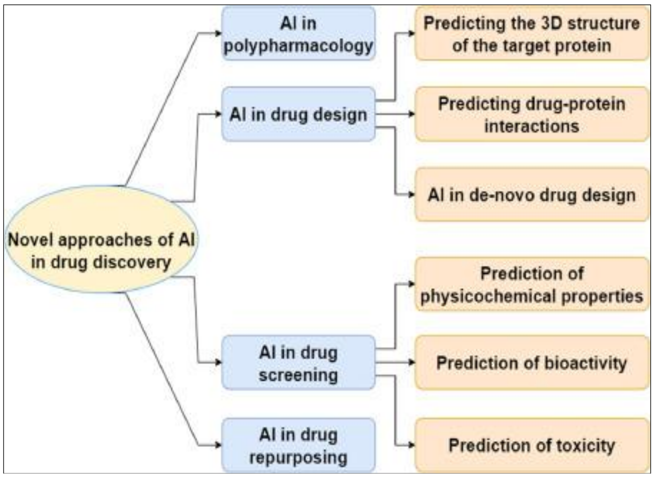

Fig 5: Applications of artificial intelligence in drug discovery

6.1 Applications of AI in drug discovery
Machine Learning (ML) has emerged as a powerful tool across the spectrum of drug discovery, offering innovative approaches to overcome traditional challenges. Its applications range from the initial stages of identifying and validating drug targets to optimizing lead compounds and assessing their safety profiles (Gaudete *et al*., 2021). This section comprehensively explores these applications, highlighting the transformative impact of ML

- **Target identification and validation**

The initial phase of drug discovery involves identifying biological targets, typically proteins, implicated in disease processes. Accurate target identification and validation are crucial for the success of subsequent drug development effortsProtein Function Prediction: Deep learning models, trained on protein sequence and structural data, can predict protein functions and interactions. This capability is instrumental in identifying proteins that play key roles in disease pathways, serving as potential drug targets.

- **Hit Discovery**

Once potential targets have been identified, the next step is to find compounds, known as "hits," that can modulate the target's activity. ML enhances the hit discovery process through virtual screening and structure-activity relationship (SAR) modelling. ML models can predict the biological activity of vast libraries of compounds against a specific target, reducing the need for extensive laboratory screening

- **Lead Optimization**

After identifying hit compounds, the next phase is optimizing these hits into lead compounds with increased efficacy, reduced toxicity, and favourable pharmacokinetic properties. ML accelerates lead optimization by predicting the properties of compound derivatives, facilitating the design of molecules with improved drug-like qualities.

7. Conclusion
Artificial intelligence and machine learning have fundamentally transformed drug discovery by enhancing the speed, efficiency, and accuracy of the process. These technologies enable rapid target identification, optimized lead discovery, and improve toxicity prediction, which together reduce development costs and timelines. Despite challenges such as data quality, in-treatability, and ethical considerations, AI holds promise for personalized medicine and saf-er, more effective treatments. Continued collaboration between researchers, industry, and regulatory bodies is essential to harness the full potential of AI and overcome remaining obstacles in the field

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