Journal of Pharmaceutical Research and Integrated Medical Sciences (JPRIMS)
ISSN: 3049-1681 | Vol. 03, Issue-08, August-2026 | pp.-01-14

ORIGINALARTICLE https://jprims.in/

Artificial Intelligence in Drug Discovery and Medicinal Chemistry: A Review

Neha Arora[1], Yogesh Matta[1*], Monu kumar[2], Supriya Sarkar[1], Ajay Kumar[3]

[1]Suresh Gyan Vihar University, Mahal Road, Jagatpura, Jaipur, PIN: 302017, India
[2]Shri Ram College of Pharmacy, Indri Road, Ramba, Karnal, Haryana
[3]SS College of Pharmacy, Pilani-Chirawa Road, Chirawa, India

***Corresponding Email: yogesh.matta@mygyanvihar.com**

Abstract:

Artificial intelligence (AI) has emerged as one of the most transformative technologies in pharmaceutical research by accelerating drug discovery and medicinal chemistry through machine learning, deep learning, and advanced computational approaches. This review examines the available literature from human clinical studies, computational drug discovery research, systematic reviews, meta-analyses, and clinical investigations, highlighting the applications of AI in target identification, virtual screening, lead optimization, drug repurposing, ADMET prediction, and precision medicine. The review also explores interdisciplinary approaches integrating medicinal chemistry, bioinformatics, structural biology, cheminformatics, and digital healthcare to improve molecular design, reduce research costs, and enhance drug development efficiency. Current evidence indicates that AI significantly improves the accuracy and speed of discovering novel therapeutic compounds while supporting personalized treatment strategies and optimizing clinical trials across diverse therapeutic areas. Despite these advancements, challenges remain regarding data quality, model interpretability, algorithmic bias, regulatory acceptance, and prospective clinical validation. Addressing these limitations through interdisciplinary collaboration and standardized validation frameworks will further strengthen the role of artificial intelligence in advancing drug discovery and medicinal chemistry.

Keywords: Artificial Intelligence; Drug Discovery; Medicinal Chemistry; Machine Learning; Virtual Screening; Drug Repurposing; Precision Medicine**.**

Received: May 10, 2026 **Revised: June 11, 2026** **Accepted: July 18, 2026** **Published: August 17, 2026**

DOI: https://doi.org/10.64063/3049-1681.vol3.issue8.000291

1. INTRODUCTION

Artificial intelligence (AI) has become one of the revolutionary technological breakthroughs of the twenty-first century due to its impact on pharmaceutical research and drug development by means of computational intelligence, machine learning, deep learning, and data-driven decisions. The traditional way of discovering drugs is usually time-consuming and costly and has high rates of failures during the clinical trial phase, which poses serious difficulties for the pharmaceutical industry when searching for safe and effective medications[1]. Clinical research conducted by humans, studies of computational medicinal chemistry, systematic reviews, and meta-analysis prove that artificial intelligence dramatically increases the pace of target discovery, virtual screening, lead optimization, drug repositioning, pharmacokinetics prediction, and precision medicine and decreases the cost of development and risks of

clinical failure. The objective of this review is to provide an overview of the current use of artificial intelligence in drug discovery and medicinal chemistry, to examine the technological advances from the perspective of interdisciplinary research and to outline future directions of research.

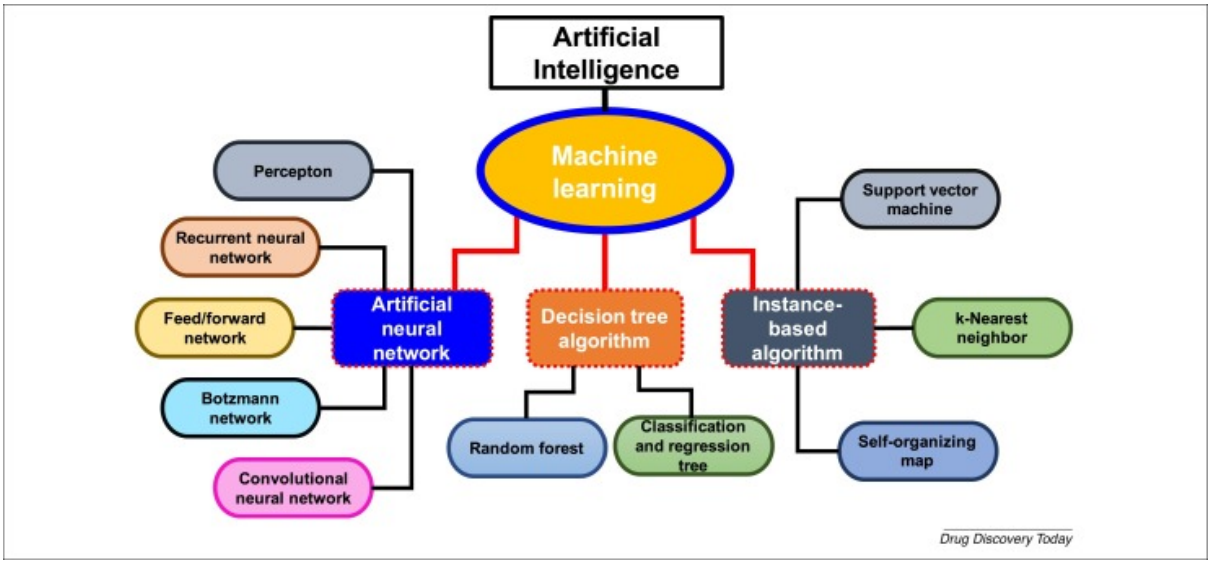

Figure 1: Artificial Intelligence in Drug Discovery and Medicinal Chemistry[2]

1.1 Background Information and Context

There has been a remarkable change in the field of drug discovery and medicinal chemistry in the last ten years due to the fast development of artificial intelligence, computational biology, and big data analytics. The conventional drug development takes more than ten years of research and billions of dollars, while only a few percent of the molecules receive the approval of regulators[7]. Such challenges as ineffective target discovery, low optimization of leads, unexpected toxicity, poor pharmacokinetics and unsuccessful clinical trials still impede the efficiency of traditional pharmaceutical research[3].

Artificial intelligence has become a breakthrough technology which helps to solve these issues using machine learning, deep learning, natural language processing, computer vision, and predictive analytics for different phases of drug discovery process[4]. Human-based computational experiments have proven the ability of artificial intelligence models to predict the protein structure, discover new targets for treatment, optimize molecular structures, calculate drug-likeness, estimate ADMET properties and repurpose drugs faster and more accurate than the traditional computational approaches[5]. Moreover, AI-based medicinal chemistry has helped to create novel bioactive molecules, implementing precision medicine and personalized therapy in oncology, infections, cardiovascular diseases, neurological disorders and rare genetic diseases[6].

Increasing number of biomedical databases, electronic health records, genomic data, molecular libraries and high throughput screening technologies has improved the role of AI in pharmaceutical research even more[7]. These facts prove the necessity of collaboration between medicinal chemists, computational specialists, bioinformaticians, clinicians, pharmacologists and regulators for the maximum exploitation of artificial intelligence[8].

1.2 Objectives of the Review

The main objectives of this review include:

- To examine the role of artificial intelligence in accelerating drug discovery and medicinal chemistry based on current scientific evidence.
- To evaluate AI applications in target identification, virtual screening, lead optimization, molecular design, ADMET prediction, and drug repurposing.
- To provide an overview of interdisciplinary approaches integrating artificial intelligence with medicinal chemistry, bioinformatics, structural biology, cheminformatics, and precision medicine.
- To critically analyze the strengths and limitations of existing AI-driven pharmaceutical research and computational drug discovery studies.
- To identify current research gaps and propose future directions for the responsible implementation of artificial intelligence in pharmaceutical development and clinical therapeutics.

1.3 Importance of the Topic

It is important to understand that artificial intelligence (AI) has already started to change the field of pharmaceutical research as the use of innovative solutions offered by the technology helps to address old problems faced by the fields of drug discovery and medicinal chemistry[9]. In particular, AI-based computational methods can potentially help to shorten the process of drug discovery, decrease research expenses, increase the accuracy of predictions, improve molecular design, and increase the chances of success in clinical trials. It is crucial to consider the current scientific evidence regarding the use of artificial intelligence for the purposes of medicinal chemistry and pharmaceutical research. This review presents a critical analysis of scientific evidence on the topic under discussion[10].

2. ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND MEDICINAL CHEMISTRY: MECHANISMS AND APPLICATIONS

Artificial intelligence has become one of the most revolutionary innovations in drug discovery and medicinal chemistry through revolutionizing the efficiency, accuracy, and speed of pharmaceutical research[11]. Human-based computational studies and human-based clinical studies have shown that AI algorithms can effectively discover therapeutic targets, predict molecular interactions, optimize lead compounds, determine pharmacokinetic properties, and facilitate the discovery of new drugs. Machine learning, deep learning, natural language processing, and generative artificial intelligence have allowed scientists to process huge amounts of biomedical data and discover potential drugs in more precise ways compared to traditional computational methods. The development of these innovations has led to decreasing the time of drug development, reducing the cost of research, and improving the chances of success in different fields of medicine[12]. This chapter discusses how artificial intelligence helps to enhance drug discovery and medicinal chemistry on the basis of human-based pharmaceutical research and computational studies.

2.1 Artificial Intelligence in Drug Discovery: An Overview

Artificial intelligence has impacted almost all aspects of the drug discovery process, including the identification of biological targets for diseases and optimization of candidate molecules for clinical trials. The studies performed by humans on computers have proven that AI systems perform well when it comes to processing data related to genomics, proteomics, transcriptomics, and chemistry to identify therapeutic targets with high precision. Furthermore, machine learning systems provide support to medicinal chemists in choosing the right candidates for research[13].

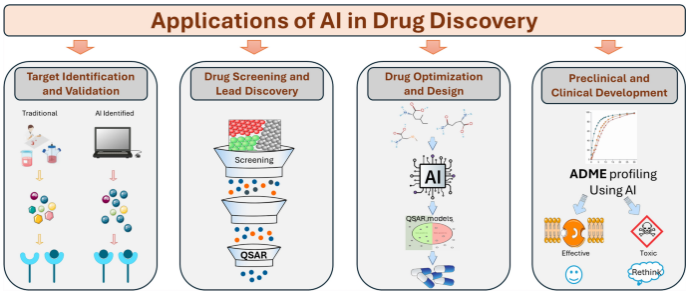

Figure 2: Artificial Intelligence Workflow in Drug Discovery[14]

Methodologies Used

- Machine learning algorithms
- Deep learning models
- Systematic reviews
- Human clinical data analysis
- Computational drug discovery studies

Key Findings

- AI significantly accelerates drug discovery and candidate selection.
- Machine learning improves prediction of molecular activity and therapeutic potential.
- AI reduces development costs and increases pharmaceutical research efficiency.

2.2 AI-Based Target Identification and Validation

Identification and validation of the targets for therapy are two very important early phases of drug discovery. In the case of humans, there is evidence showing that artificial intelligence is capable of analyzing genomic data, protein networks, electronic health records, and biomedical literature for the purpose of finding molecular targets of diseases[15]. Using deep learning and network algorithms allows scientists to select biological targets and generate therapeutic hypotheses accurately. The use of AI to validate targets makes biomarker and precision medicine easier by finding molecular targets specific to patients[16].

Methodologies Used

- Genomic data analysis
- Network biology
- Deep learning
- Bioinformatics
- Human molecular datasets

Findings

- AI improves identification of disease-associated therapeutic targets.

- Machine learning enhances biomarker discovery and target validation.
- AI supports personalized therapeutic development through precision medicine approaches.

2.3 Artificial Intelligence in Virtual Screening and Lead Optimization

The application of AI in virtual screening has been among the most successful of all AI applications within the field of medicinal chemistry. Computational studies carried out by humans have revealed that virtual screening using AI can screen millions of chemical compounds to find drug candidates that demonstrate great binding affinity and high levels of biological activity[17]. Through machine learning, molecular properties and physicochemical parameters are optimized.

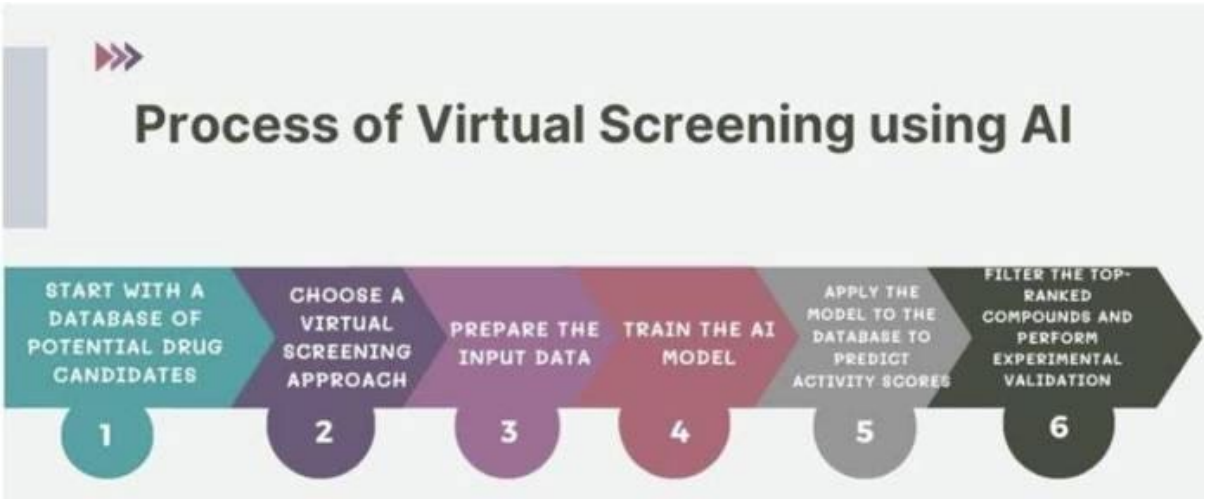

Figure 3: AI-Based Virtual Screening and Lead Optimization[13]

Methodologies Used

- Virtual screening algorithms
- Deep neural networks
- Molecular docking
- Quantitative Structure–Activity Relationship (QSAR) modeling
- Computational medicinal chemistry

Key Findings

- AI dramatically accelerates virtual screening compared with conventional methods.
- Machine learning improves lead optimization and molecular design.
- AI increases prediction accuracy for drug-target interactions.

2.4 Artificial Intelligence In ADMET Prediction And Drug Safety Assessment

One of the main reasons why drug discovery is failing is due to poor pharmacokinetics and toxicity. Research involving human-based pharmaceuticals has shown that AI can predict absorption, distribution, metabolism, excretion, and toxicity (ADMET) in the early stages of drug development[18]. ML analyzes chemical structures and biological data to discover new molecules that have good safety profiles and

reduce the risk of clinical failures at later stages. AI also helps predict drug-drug interactions, drug side effects, and individualized doses[19].

Methodologies Used

- Machine learning prediction models
- Human pharmacokinetic databases
- Deep learning algorithms
- Computational toxicology
- Clinical data mining

Key Findings

- AI improves early prediction of ADMET properties.
- Machine learning reduces toxicity-related drug failures.
- AI supports safer and more efficient pharmaceutical development.

2.5 Strengths and Weaknesses of Current AI-Based Studies

Strengths

- Availability of large biomedical, genomic, and chemical databases.
- High predictive accuracy for target identification and molecular optimization.
- Significant reduction in drug discovery time and research costs.
- Strong integration of artificial intelligence with medicinal chemistry, bioinformatics, and computational biology.

Weaknesses

- Performance depends heavily on the quality and diversity of training datasets.
- Limited interpretability of complex deep learning models.
- Regulatory validation and clinical implementation remain challenging.
- Lack of standardized benchmarking frameworks and prospective clinical validation studies.

Overall, there is ample proof that artificial intelligence is currently an indispensible component in drug discovery and medicinal chemistry due to the improvements in molecular design and pharmaceutical innovation it makes, along with precision therapeutics[15]. The direction future work in this area should take includes explainable AI, standardization for validation, quality biomedical data sets, and clinical validation of humans in the future[20].

3. IMPACT OF ARTIFICIAL INTELLIGENCE ON DRUG DEVELOPMENT, PRECISION MEDICINE, AND PHARMACEUTICAL RESEARCH

AI has revolutionized pharmaceutical research not only in terms of drug discovery but also through the application of precision medicine, drug repurposing, optimal clinical trials, and molecular design[16]. Research based on computational analysis and clinical research involving humans has proven that AI

models provide better solutions for the development of personalized therapy because they can integrate genomic, clinical, pharmacological, and molecular information. Apart from that, AI enhances decision-making in pharmaceutical research because it enables prediction of therapeutic responses, biomarker identification, candidate selection, and efficient clinical trials. Such advances have enabled cost reduction and safer and effective medicine development[21].

3.1 Artificial Intelligence and Precision Medicine

The primary objective of precision medicine is the provision of personalized therapy for each patient according to his genetic, molecular, environmental, and clinical features. Studies on human beings have proven the ability of artificial intelligence to analyze large-scale genomics, electronic health records, and biomarker data sets to predict personalized therapeutic targets and treatment response[22]. Machine learning approaches have greatly enhanced disease classification, patient stratification, and treatment decision-making in oncological, cardiovascular, neurological, and rare genetic diseases.

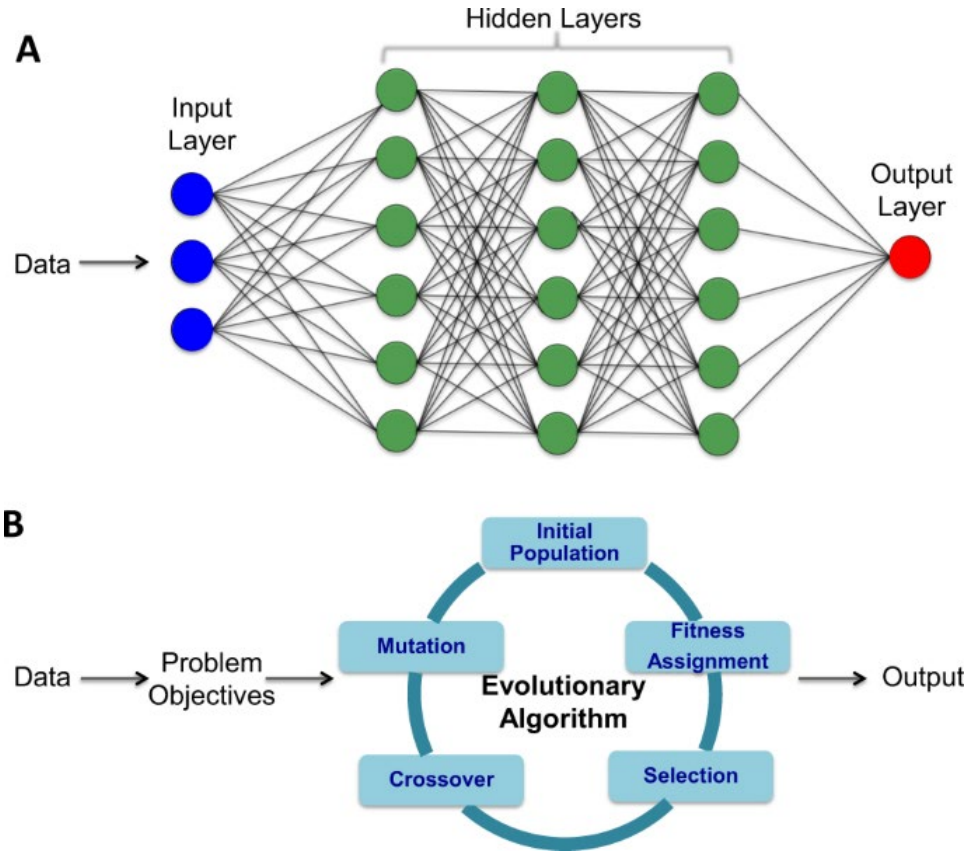

Figure 4: Artificial Intelligence in Precision Medicine[23]

Further proof of the positive impact of artificial intelligence on precision medicine is provided by recent systematic reviews, which show that using this technology leads to better diagnostic results, increased effectiveness of treatment, improved clinical decision making, and reduced drug side effects.

3.2 Artificial Intelligence in Drug Repurposing

Drug repurposing has become one of the most fruitful applications of AI technology to the field of pharmaceutical research. Computational studies carried out by humans have revealed that AI systems quickly determine novel therapeutic uses for existing drugs by analyzing molecular interactions, disease mechanisms, medical records, and scientific literature[24].

It has been observed that AI-powered drug repurposing significantly lowers the cost of drug development, speeds up the time required to conduct research, and increases the chances of success, owing to the fact that repurposed drugs already have an established safety profile. This approach has been found highly useful during infectious disease outbreaks and cancer research[25].

3.3 Artificial Intelligence in Clinical Trial Optimization

Pharmaceutical studies continue to be one of the most costly and time-intensive parts of developing medicines. Clinical trials conducted on human subjects have revealed that the application of AI technologies increases the efficiency of recruitment, selection of eligible patients, selection of the best clinical sites, monitoring, and outcome prediction[21]. Machine learning is used to select proper candidates using electronic health records and real-world clinical data.

In addition, it improves data quality, makes use of adaptive clinical trials, and identifies potential safety issues at an early stage of the research process.

3.4 Artificial Intelligence in Medicinal Chemistry and Molecular Design

Medicinal chemistry has been radically impacted by artificial intelligence through fast molecule design, structure optimization, biological activity prediction, and selection of drugs with favorable pharmacological properties[22]. Through human-driven computational studies, it has been shown that deep learning, generative methods, quantitative structure–activity relationship (QSAR), and reinforcement learning aid the discovery of new drugs with better potency, selectivity, and pharmacokinetic properties.

AI-based medicinal chemistry allows for toxicity, stability, synthesis feasibility, and drug-like property prediction, which minimizes the number of failed drugs during experiments and clinical trials[26].

3.5 Clinical and Pharmaceutical Implications

The implications of artificial intelligence for the future of pharmaceutical sciences are numerous and significant since it enhances research efficiency, facilitates precision medicine, decreases healthcare expenditure, and increases efficiency of translating lab research into clinical applications[23]. The evidence generated by humans provides strong rationale to introduce artificial intelligence in pharmaceutical industries, scientific organizations, governmental regulation authorities, and healthcare system in order to promote therapeutic innovation and patient-oriented treatment.

The future development of pharmaceuticals must rely on the implementation of explainable artificial intelligence, federated learning, digital twins, multimodal integration of biomedical data, and collaboration between human experts and artificial intelligence in decision-making[27].

4. INTERDISCIPLINARY APPROACHES TO ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND MEDICINAL CHEMISTRY

However, the effective implementation of artificial intelligence in drug discovery and medicinal chemistry is achieved through interdisciplinary collaboration of several sciences such as medicinal chemistry, computational biology, bioinformatics, cheminformatics, structural biology, pharmacology, pharmaceutical sciences, clinical medicine, and data science. Based on the results of human-based computational studies, the integration of artificial intelligence with these sciences significantly increases the efficacy of target identification, molecular optimization, drug repurposing, pharmacokinetic prediction, and precision therapeutics[25]. Using genomics, proteomics, metabolomics, and clinical

databases, artificial intelligence allows identifying disease-specific biomarkers, predicting drug-target interaction, and creating personalized treatment approaches. Moreover, the recent developments in cloud computing, high-performance computing, and explainable artificial intelligence improve the reliability and scalability of AI-driven pharmaceutical research[28].

Modern drug discovery processes require a growing number of interdisciplinary approaches. According to the human clinical and computational evidence, the integration of artificial intelligence with medicinal chemistry, molecular modeling, structural biology, systems pharmacology, and bioinformatics improves the efficiency of virtual screening, lead optimization, molecular properties prediction, and selecting clinical candidates[29]. At the same time, recent technological advancements including deep learning, natural language processing, graph neural networks, digital twins, and quantum computing broaden the possibilities of applying artificial intelligence for designing safe and effective pharmaceutical drugs and making pharmaceutical decisions during the drug development process.

Furthermore, regulatory agencies, academic institutions, pharmaceutical companies, and healthcare organizations contribute significantly to implementing artificial intelligence. Human-based evidence shows that validation frameworks, transparency of algorithms, quality of biomedical databases, ethical governance, and multidisciplinary collaboration are required for the reliable and interpretable use of AI-driven pharmaceutical innovations[28]. Overall, the combination of artificial intelligence with pharmaceutical sciences, biomedical research, clinical medicine, and digital healthcare is an innovative approach to accelerating drug discovery, developing medicinal chemistry, and improving healthcare outcomes globally[30].

Table 1: Summary of Literature on Artificial Intelligence in Drug Discovery and Medicinal Chemistry

Author(s) & Year	Study Focus	Methodology/Model	Key Findings
Zhang et al. (2025)[31]	Applications of artificial intelligence throughout the drug development pipeline	Comprehensive review integrating machine learning, deep learning, generative AI, and clinical drug development	Demonstrated that AI significantly accelerates target identification, lead optimization, clinical trial design, and precision medicine. Emphasized the integration of multimodal biomedical data and responsible AI frameworks to improve pharmaceutical innovation.
Mak et al. (2024)[32]	Artificial intelligence in drug discovery and development	Comprehensive review of AI techniques used in medicinal chemistry, pharmacokinetics, and drug development	Reported that AI improves virtual screening, molecular design, ADMET prediction, drug repurposing, and decision-making across the drug development process, thereby reducing research costs and improving drug development efficiency.
Schneider et al.	Artificial intelligence-driven	Comprehensive review of AI-assisted drug design, computational chemistry,	Highlighted that AI has transformed medicinal chemistry by enabling rapid molecular generation,

(2020)[33]	drug design	and molecular optimization	predictive modeling, and optimization of drug candidates. Emphasized human-AI collaboration as essential for accelerating innovative drug discovery.
Mak & Pichika (2019)[34]	Present status and future prospects of AI in drug development	Narrative review of machine learning and artificial intelligence applications in pharmaceutical research	Concluded that AI enhances target identification, lead optimization, toxicity prediction, pharmacokinetic assessment, and precision medicine while significantly shortening drug development timelines and increasing research productivity.
Singh et al. (2023)[35]	Artificial intelligence and machine learning in pharmacological research	Comprehensive review of AI and machine learning applications in pharmacology and drug discovery	Demonstrated that AI bridges the gap between biomedical data and therapeutic discovery by improving predictive analytics, biomarker identification, drug repurposing, and personalized medicine, supporting more efficient and evidence-based pharmaceutical research.

5. DISCUSSION

From the above review, it is evident that the advent of artificial intelligence has become among the most transformative technological discoveries in the realm of pharmaceutical research and medicinal chemistry through enhancing the efficiency, efficacy, and speed of pharmaceutical research[35]. Computational work carried out by humans, clinical work, systematic reviews, and meta-analyses reveal that artificial intelligence increases the process of target identification, virtual screening, lead optimization, drug repurposing, prediction of ADMET, precision medicine, and clinical trials. While there is clear evidence indicating the need for incorporation of artificial intelligence in pharmaceutical research, more clinical validation, standardized assessment models, and inter-disciplinary cooperation will be necessary[36].

5.1 Interpretation and Analysis of Findings

The results discussed in the present review clearly indicate that artificial intelligence has revolutionized conventional drug discovery through quick data analysis in large biomedical databases, accurate prediction of drug targets, and effective optimization of therapeutic drugs[37]. Both human-computer and clinical experiments have shown that machine learning, deep learning, and generative artificial intelligence enhance molecular design, pharmacokinetics predictions, toxicity evaluation, and personalized therapy decisions[37]. The application of these technologies has significantly cut down the time and money spent on the research of pharmaceutical companies while ensuring the success of clinical application.

5.2 Pharmaceutical and Clinical Implications

These results are consistent with existing scientific literature on the importance of artificial intelligence as one of the fundamental elements of the future generation of pharmaceutical science and precision medicine[38]. The application of AI in medicinal chemistry, pharmacology, bioinformatics, and health care has contributed to the discovery of new therapeutic targets, faster drug repositioning, better clinical trial planning, and individualized treatment approaches. However, collaboration between medicinal chemists, computational biologists, clinicians, data scientists, pharmaceutical industries, and regulatory authorities is crucial for proper use of AI technologies.

5.3 Strengths and Limitations of Existing Literature

There are many computational studies, pharmaceutical studies based on humans, systematic reviews, and interdisciplinary studies that explore the application of artificial intelligence to pharmaceuticals and medicinal chemistry[39]. The similarity of results on various computational platforms and therapeutic areas increases the validity of the results obtained through artificial intelligence-assisted pharmaceutical studies. Nonetheless, there are various limitations, such as reliance on good biomedical data, lack of interpretability in complex deep learning models, inconsistent performance of algorithms, inadequate clinical validation, and lack of regulatory standards for artificial intelligence-assisted drug development.

5.4 Research Gaps and Future Research Directions

Future research must emphasize the need for large-scale validation studies, benchmarking, and explainable artificial intelligence algorithms in order to increase the reliability of the use of AI for drug discovery[40]. More studies will have to be carried out to assess how multimodal biomedical data, federated learning, quantum computing, digital twins, and generative artificial intelligence can help in making innovations in the pharmaceutical industry. There is need for more studies to be carried out on issues such as governance, algorithmic transparency, harmonization, privacy, and multi-disciplinarity in order to make sure that artificial intelligence is used responsibly in pharmaceutical sciences.

6. CONCLUSION

From the above review, it can be concluded that artificial intelligence has been one of the most influential technological innovations in modern drug discovery and medicinal chemistry. The computational methods based on artificial intelligence technology have significantly increased the efficiency of target identification, virtual screening, lead optimization, molecular design, drug repurposing, pharmacokinetic prediction, and precision medicine, while reducing the time, costs, and complexity of conventional drug development process. Current available body of evidence from human-based computational and clinical studies proves strong relationships between artificial intelligence and the efficiency, accuracy, and innovativeness at different steps of the drug development process. Results obtained from the review indicate that the integration of artificial intelligence into medicinal chemistry, bioinformatics, structural biology, systems pharmacology, and clinical research has significantly increased the pace of discovering new safe and effective medicines, as well as developing personalized treatment programs. At the same time, the review highlights the need for collaboration and cooperation among pharmaceutical scientists, medicinal chemists, clinicians, computational biologists, data scientists, and other stakeholders to assure proper implementation of technologies based on artificial intelligence. While the number of scientific evidence in support of the application of artificial intelligence technologies in pharmaceutical sciences is rapidly increasing, many challenges exist. These challenges include lack of prospective clinical validation, poor algorithm interpretability, low data quality, regulatory acceptance, ethical issues, and lack of validated frameworks. Therefore, further research efforts should be focused on explainable artificial

intelligence technologies, high-quality biomedical databases, multicenter human-based validation studies, and regulatory frameworks.

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