INTERNATIONAL JOURNAL OF PHARMACEUTICAL SCIENCES
[ISSN: 0975-4725; CODEN(USA): IJPS00]
Journal Homepage: https://www.ijpsjournal.com

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Review Article

From Bench to Bedside: How Artificial Intelligence is Reshaping Drug Discovery and Clinical Trials

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ARTICLE INFO

Published: 30 Aug 2025
Keywords:
Drug Discovery, Artificial Intelligence, AI Algorithms, Clinical Trial Design, Drug Repurposing, Personalized Medicine, Challenges.
DOI:
10.5281/zenodo.17008073

ABSTRACT

" AI is likely to be either the best or worst thing to happen to humanity." -Elon Musk. AI has started to improve its application across different sectors, with the pharmaceutical industry gaining the most benefits, especially in drug discovery, development, and clinical trials by reducing human effort, time, and costs while increasing success rates.AI employs machine learning, deep learning, and natural language processing to analyze large datasets, enabling the rapid identification of drug targets, predicting compound efficacy, and enhancing drug design. Many drug molecules have been discovered through AI-based methods and tools, with several of these newly identified compounds already advancing to clinical trials. This review provides a comprehensive analysis of how AI is transforming the drug discovery and development field, emphasizing its contributions to target identification, virtual screening, drug design, and the optimization of clinical trials. Additionally, we have explored the major challenges and limitations that need to be addressed, such as data quality, model interpretability, regulatory hurdles, data standardization, transparency in AI model development, and the necessity for improved collaboration between AI researchers and pharmaceutical experts.

INTRODUCTION

The process of drug discovery and development consists of three primary phases: the discovery of the drug, the preclinical development of drug compounds, and the clinical development of the therapeutic agent. The process of discovering a drug is intricate and costly, often resulting in a significant failure rate. A high level of expertise and various technologies have been used in drug discovery. Developing a new drug typically costs over $2.6 billion on average and can take more

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Relevant conflicts of interest/financial disclosures: The authors declare that the research was conducted in the absence of any commercial or financial relationships that could be construed as a potential conflict of interest.

than a decade to complete[1] . This process, known as from bench to bedside.

Furthermore, merely a tiny percentage of drug candidates that proceed to clinical trials eventually obtain Regulatory approval. In spite of ongoing efforts, just 2.01% of drug development initiatives culminate in a successful marketable drug. These obstacles underscore the pressing necessity for innovative strategies to enhance and expedite the success rates of drug discovery[2] .

A recent analysis of drug development expenses revealed that the capital cost associated with drug development is US$1.3 billion . Concurrently, the average out-of-pocket cost for successful drug development is merely US$200 million. In contrast, the out-of-pocket costs incurred from failures amount to US$1 billion[2]. Consequently, the overall cost of successful drug discovery can be lowered by minimizing the costs associated with failures. The expenses related to failures in drug discovery can potentially be decreased through the implementation of advanced technologies such as AI . Meanwhile, traditional methods remain suboptimal for discovering new drugs for various diseases[3] [4] [5] .

Most of the AI-discovered molecules are currently in Phase I trials, although some have already progressed to Phase II and beyond. These molecules represent a broad range of therapeutic areas, with oncology particularly prominent, accounting for 50% of AI-discovered molecules in Phase I and Phase II[6] [5] .

As of December 2023, 24 AI-discovered molecules had completed Phase I trials, of which 21 were successful. This suggests a success rate of 80–90%, which is substantially higher than historical industry averages that range from 40% to 55– 65%. When we break out the Phase I data by mode of discovery, we see similar results across the board[7]

In Phase II, ten AI-discovered molecules have completed trials, of which four were successful. This implies a success rate of 40%, which is in line with historical industry averages of 30–40%[6] [2]

The main aims and objectives of this study are: 1. To present a comprehensive examination of how artificial intelligence is altering drug discovery and development, with a focus on target identification, virtual screening, drug design, and clinical trial optimization.2. To explore the major challenges and limitations that need to be addressed, such as data quality, model interpretability, regulatory hurdles, data standardization, transparency in AI model development, and the necessity for improved collaboration between AI researchers and pharmaceutical experts[8] [9] [10] [6]

METHODOLOGY/ SEARCH STRATEGY:

To find pertinent studies published between 2022 and 2025, we thoroughly searched several databases, including PubMed, SCOPUS, Google Scholar, and the Research Gate platform. This timeframe was chosen to align with the period when contemporary AI models started to be used extensively in experiments. "Artificial intelligence," "clinical intelligence," and "clinical trials" were the free-text search terms we employed. To locate more articles, we also manually examined the references of relevant publications. By using this approach, we were able to compile pertinent research on the use of AI in data mining, pre-clinical research, and clinical trials, among other phases of drug discovery and development.

OVERVIEW OF ARTIFICIAL INTELLIGENCE

Artificial intelligence (AI), often known as machine intelligence, governs computer systems' capacity to learn from past data and input. Various artificial intelligence methods have been utilized across multiple domains of drug discovery, such as virtual screening, target identification, and hit-to-lead development. Additional applications encompass bioavailability forecasting, retrosynthetic analysis, and reaction prediction, along with de novo drug discovery[5] [11] [12] . The discovery and development of drugs depended on the process of producing numerous models. Model designs have therefore evolved as well to reduce the influence of the healthcare industry. There have also been improvements in model architectures, including graph NNs, transformers, convolutional neural networks (CNNs), and recurrent neural networks (RNNs [13] [12]

Algorithms used for AI and ML

Numerous algorithms pertaining to artificial intelligence have been created for the purpose of finding and developing new drugs. With the aid of AI-enabled algorithms or methodologies utilizing various data resources, drug discovery and related tasks are completed extremely quickly.

In AI-enabled drug discovery and development, two categories of AI algorithms or approaches are frequently employed: supervised and unsupervised learning algorithms or techniques. Apart from these techniques, multiple linear regression is a modeling regression analysis algorithm that is frequently utilized[14] [6] [15] [13] . Machine Learning (ML) is a key paradigm in artificial intelligence, which includes a variety of domains such as knowledge representation, reasoning-based domains, and solution search domains. ML is hence considered a subfield of AI. Similarly, deep learning (DL) shows promise as a branch of machine learning. Artificial Neural Network (ANN) techniques are included in DL. Recurrent neural networks (RNNs), multilayer perceptron networks, and convolutional neural networks (CNNs) are only a few of the many types of artificial neural networks (ANNs) .

AI IN DRUG DISCOVERY & DEVELOPMENT

Target identification and validation.

AI improves medication target prediction by examining a wide range of biological data. Through the integration of proteomics, genomes, and other sources, AI algorithms can find novel targets more successfully than conventional techniques . AI is capable of analyzing genomic data, for instance, to find genetic variants linked to illnesses and to pinpoint genes and the proteins they encode as possible targets. Proteomic data, including protein interactions and structures, can also be analyzed by AI to determine which proteins are implicated in disease pathways and evaluate their druggability[5] [2] . Artificial Intelligence can additionally integrate various data sources, including DrugBank, PubChem, and the Antibiotic Combination Database (ACDB)[5] .

Design of medicinal compounds utilizing ML and DL.

Drug molecular design is an important element of drug development, and ML and DL algorithms have aided in the structural design of medicinal molecules. RNNs and autoencoders are examples of deep learning algorithms used in molecular design during drug discovery and development[16] . Molecular graphs and 3D geometric models are two methods that can be used to represent molecules in the development of medicinal compounds.SMILES and string-based representations, image-based representations, tensor representations, and other graph-based

representations can all be used to refine molecular graph representations[17]

Drug screening and lead discovery

AI-powered virtual screening, and in silico techniques have transformed the identification of possible lead compounds in drug research. These methods use computational algorithms to rapidly evaluate enormous chemical libraries, considerably speeding up the procedure and lowering expenses when compared to traditional high-throughput screening[14] [18] . These techniques rely heavily on machine learning algorithms. For example, they can be used to build quantitative structure-activity relationship (QSAR) models that predict the biological activity of substances based on their chemical structures. These models can then be used to screen vast chemical libraries and prioritize compounds that have the best chance of binding to the target of interest[18] .

Drug optimization and design

Because AI-driven methods optimize vital characteristics like solubility, stability, and bioavailability, they are transforming the medication development process. ML algorithms can examine massive datasets of chemical structures and their associated properties in order to predict critical parameters with high accuracy[11] . For example, QSAR predictions used around 1000-5000 data points to estimate water solubility, whereas DL models can predict drug stability under a variety of situations. Protein sequence data from many species can be collected by researchers utilizing two open databases: the UniProt Consortium and the Protein Data Bank (PDB), which are used to predict protein function[18] .

Prediction of drug toxicity

Drug toxicity assesses the undesirable or adverse effects associated with drug-like molecules. It plays a significant role in the expensive process of drug development. This characteristic is closely linked to drug safety. In the course of drug development, predicting side effects and measuring drug safety are crucial elements[19] . However, laboratory assessments of drug toxicity during the development phase can be quite time-consuming. As a result, computational models help to save both time and costs in this regard. Recently, a three-layer deep neural network (DNN) model named DeepTox was created to predict the toxicity of drug-like compounds. Additionally, a deep learning-based toxicity prediction model called Deep-PK has also been developed. ClinTox, ToxCast, and Tox21 are examples of data-driven databases and libraries used for toxicity prediction [20] .

Artificial intelligence in lead optimization.

Lead optimization is a critical stage in drug discovery in which the structure of a lead chemical is fine-tuned to increase efficacy, reduce toxicity, and improve pharmacokinetic properties. AI contributes significantly to lead optimization by anticipating how changes to a chemical structure will affect its overall drug-like properties. Molecular dynamics (MD) simulations with AI[6] [21] [4] [15] . AI improves MD simulations by providing more precise predictions of how molecules would behave in different physiological conditions. MD simulations are used to determine a drug's stability while attached to its target, as well as how it interacts with biological membranes, enzymes, or transporters[22] [23] .

With the help of machine learning methods like random forests, support vector machines (SVMs), and neural networks, AI-driven QSAR models are able to generate extremely accurate predictions for new compounds by drawing on vast databases of

chemical structures and the activities that go along with them.

AI in preclinical and clinical development (clinical trials)

Preclinical and clinical research are being transformed by artificial intelligence to become more efficient, have lower failure rates, and create new drugs more quickly. Extensive experimentation, expensive clinical trials, and high failure rates due to unforeseen toxicity or insufficient efficacy are characteristics of traditional research methods[24] [25] [14] . A complex strategy that keeps transforming many facets of clinical research is the incorporation of AI and ML into clinical trials. These technologies offer a wide range of tools for accelerating the development of new medical therapies in a patient-centric way, from patient recruitment to real-time adaptation, predictive modeling, and ensuring ethical behavior[24] [5] [9] [14] [26] .

AI-powered digital twins can simulate virtual patient populations by anticipating treatment outcomes and eliminating the need for huge control groups, resulting in speedier and more precise clinical studies.DeepDrug (eMolFrag, eSynth, eToxPred, eDrugRes, eVir, eComb) and BenevolentAI (knowledge graphs and protein pocket analysis) are among the AI teams working on clinical trial themes. By 2024, Exscientia had grown, with six AI-designed compounds starting clinical trials. These include immunological, psychological, and oncological therapy[27] [5] .

Clinical trial design

Clinical trial design is another area where AI is making a huge impact. Clinical trials are typically the most expensive and time-consuming phase of drug development, and many promising medicines are derailed by poor study design, patient selection, or adverse effects.

Artificial intelligence enhances research efforts by analyzing patient data, identifying appropriate individuals, and assessing treatment outcomes. Machine learning algorithms can classify patient groups based on genetic, clinical, and demographic characteristics, making it easier to conduct trials with individuals who are most likely to benefit from the treatment[28].

Adaptive trial designs that use AI can modify dosage, treatment length, and even patient enrollment in real time based on results. This adaptive strategy maximizes trial success and speeds up approval.

Natural Language Processing (NLP) methodologies facilitate the rapid retrieval of information from medical literature, clinical documentation, and various textual sources, thereby expediting the design and conceptualization of trials. AI/ML uses data mining, predictive modeling, natural language processing (NLP), and machine learning algorithms to help design new clinical trials [6] [29] [14] .

Recruitment

The recruitment of suitable patients can assure the success of a clinical trial, which would otherwise result in 86% failure. AI can help select only a certain diseased population for recruitment in Phase II and III clinical trials by analyzing patient-specific genome-exposome profiles, which can aid in the early prediction of possible therapeutic targets in the patients selected[6] .

The recruiting of patients comprises around 33% of the clinical trial's duration. Appropriate case registration can help a clinical trial succeed, but it

can also lead to a non-fruition outgrowth in roughly 86% of cases.

Patients dropping out of clinical trials account for 30% of trial failures, necessitating further recruiting for study completion, resulting in a waste of time and money. This can be avoided by closely monitoring the participants and assisting them in following the intended clinical trial protocol. AiCure developed mobile software to track regular medication intake by schizophrenia patients in a Phase II trial, which boosted patient adherence by 25% and ensured the clinical trial's success.

AI-designed molecules entering clinical trial:

The earliest results for AI-designed compounds are encouraging. Some AI-designed medicines have passed the preclinical stage and entered clinical trials. EXS-21546, an AI-designed A2A receptor antagonist chemical, has also entered clinical trials. This immuno-oncology medication will be used to treat solid tumors that have increased adenosine signatures.

It resulted from a collaborative effort between Evotec and Exscientia. Exscientia AI Ltd. is a renowned pharmaceutical technology business that does AI-based medication discovery. Evotec is a biotechnology drug discovery business established in Germany. molecules in both Phase I and Phase II.

Post-Marketing Safety Monitoring.

During the post-approval phase, the reporting of adverse events associated with drug use is an integral component of post-marketing safety monitoring, also referred to as pharmacovigilance (PV) activities. Pharmacovigilance refers to the methods and studies involved in detecting, assessing, understanding, and preventing adverse events or other drug-related difficulties (such as medication errors and product quality problems). Adverse events occurring after a product's market introduction are communicated to the FDA through an individual case safety report (ICSR). It is essential to ensure that ICSRs are reported completely and accurately to gain insights into a drug's safety profile [30] .

Artificial Intelligence in pharmacovigilance plays a vital role in the prompt detection and reporting of adverse drug reactions, thereby enhancing patient safety throughout clinical trials. The FDA is investigating the use of AI and machine learning applications to assist regulatory agencies in the processing and assessment of ICSR submissions, with the expectation of a substantial rise in the volume of ICSR reports[30] .

Personalized medicine approaches

The emergence of personalized medicine is one of the most intriguing uses of artificial intelligence (AI) in drug discovery. The treatment paradigm for diseases and the process of drug development are transitioning towards personalized therapies, aiming to yield improved outcomes for individual patients.

AI facilitates the creation of customized drug formulations that cater to the specific needs of individual patients, taking into account genetic, lifestyle, and medical factors. Furthermore, AI tackles the challenge of providing adaptable dosage strengths, which is essential for medications with a narrow therapeutic index, through innovations such as data-enhanced edible pharmaceuticals.

In conclusion, by enhancing preclinical research, honing clinical trial procedures, and customizing treatment plans for each patient, the application of

AI in drug development holds the potential to revolutionize the pharmaceutical industry.

Drug repurposing

The creative process of drug repurposing, which uses previously approved drugs to find new therapeutic applications for them, is increasingly utilizing artificial intelligence (AI). Repositioning existing approved medications offers a faster and more cost-effective alternative by leveraging pre-existing safety and efficacy data[31] . Drugs typically possess multiple molecular targets, and AI models can systematically investigate these targets to uncover new therapeutic activities . By employing machine learning algorithms trained on genomic, proteomic, and clinical data, researchers can forecast whether a drug initially developed for one condition can potentially be repurposed for another. When it comes to finding medicines for orphan diseases, where conventional drug discovery techniques are frequently not financially viable, this process has been especially successful[32] [1] .

Several successful instances underscore the promise of AI-enhanced drug repurposing in tackling significant medical challenges. During the COVID-19 pandemic, AI was employed to identify existing drugs with antiviral properties and rapidly screen them as potential candidates, such as remdesivir and baricitinib[32] .

Artificial Intelligence Applications in Drug Repurposing: Several AI-driven methods, such as PREDICT,775 SLAMS,776 NetLapRLS, and DTINet, have been proposed to find possible drug repurposing opportunities by combining data from diverse heterogeneous sources[32] .

Challenges and Ethical Considerations

The integration of artificial intelligence in drug discovery presents significant opportunities, yet it also brings forth considerable challenges and ethical dilemmas. As AI technologies evolve, it is essential to address issues related to data privacy, bias, explainability, and regulatory compliance to ensure the ethical application of these technologies in medicine[1] [9] [33] [15] .

DATA SECURITY AND PRIVACY:

Data security and privacy are two of the key problems in AI-driven drug discovery algorithms require vast amounts of biomedical, genomic, and patient data to make accurate predictions and optimize drug development processes[6] [9] [15] . Handling medical data raises issues of confidentiality and the risk of unauthorized access. Implementing robust data encryption, secure storage solutions, and compliance with privacy regulations such as GDPR and HIPAA necessitates stringent practices to maintain patient trust. Additionally, the use of anonymized or synthetic data can help reduce privacy risks while allowing AI to extract valuable insights[34] .

DATA QUALITY AND AVAILABILITY:

The limited availability of data presents a major obstacle to the advancement of AI in healthcare, especially concerning small sample sizes and privacy issues. Ensuring the quality and reliability of the data utilized for training AI models is vital for making accurate predictions and informed decisions. The biggest problem is finding high-quality datasets that are also adequate for training models. While the volume of chemical and biological data is on the rise, the quality remains subpar. Consequently, data curation is necessary. Furthermore, accessing data from databases incurs additional costs for companies, potentially increasing drug development expenses. But it's

very important that more high-quality datasets are available in pharmacology.

BIAS IN AI MODELS:

Inaccuracies, biases, and incomplete data can result in flawed outcomes. AI models may adopt the biases found in their training data, which can lead to skewed predictions or decisions. This issue is especially critical in healthcare, where biases related to race, gender, or socioeconomic status can affect patient outcomes. It is vital to develop methods for identifying and reducing biases in AI models, as well as to ensure that training datasets are diverse and representative, to uphold ethical standards in drug discovery.

INTERPRETABILITY AND TRANSPARENCY OF AI OR DL MODELS:

AI or DL-based models for drug discovery and development must be thoroughly understood and explained. A significant barrier to the widespread use of AI systems is their inherent complexity and lack of clarity. Many AI models, particularly deep neural networks (DNNs), operate as "black boxes," making it difficult to interpret the rationale behind their decisions[9] [6] [15] . The absence of interpretability and transparency brings forth concerns about trust, accountability, and the potential for unintended bias. For example, in healthcare, clinicians need to comprehend the reasoning behind an AI-generated diagnosis to make informed decisions and ensure patient safety. There is an increasing demand for interpretable AI models, where domain experts and regulatory bodies can grasp the reasoning behind predictions or recommendations. Establishing systems to ensure accountability for AI-driven decisions, including transparency in model training and validation, is essential for upholding ethical standards in drug discovery[30]

Highly skilled professionals and trained personnel

With expertise in both fields, such as computer engineering with a focus on AI and knowledge of pharmaceutical sciences, are urgently needed. These competencies facilitate the modification of algorithms in this area and enable the understanding and prediction of algorithmic outcomes in pharmaceutical science and drug development. They may address the challenge of interpretability in AI models. Similarly, the models created using AI techniques often lack explainability. Additionally, the results derived from AI cannot be clarified due to their black box nature [10] [32] [1] [15] [6] [30] [11] [9] .

Conventional pharmaceutical workflows:

They are typically defined by strict protocols and a significant focus on established practices. The integration of AI may necessitate considerable modifications to the current infrastructure, workflows, and skill sets. Additionally, issues related to data privacy, intellectual property, and the possible effects of AI on employment in the pharmaceutical sector can obstruct the implementation of these technologies [34] .

Computational Constraints

Computational constraints on sophisticated AI models. Since these advanced AI models require extensive training with massive amounts of data, smaller research institutions cannot afford them. Large amounts of processing power and storage are required to run these models. Advanced AI models may benefit from parallel computing. Large research organizations need a lot of storage space in this approach; thus, every nation should build a sophisticated computational infrastructure[15] . Infrastructure can be too expensive; thus, not all organizations may decide

to construct it. Therefore, the government ought to assist the businesses. However, organizations conducting AI-enabled drug research must have access to top-tier infrastructure. It could fix infrastructure issues related to high-end AI models' computational limitations [10] .

Ethical and Compliance Challenges to AI's Expanding Role in Clinical Trials

The ethical considerations surrounding AI continue to be a significant concern in AI-driven biopharmaceuticals. Particularly in intricate fields like cell and gene therapy, probability-based analytics frequently conflict with conventional deterministic methods, posing challenges for their implementation. Unresolved biases within AI systems can worsen inequalities in disease diagnosis and medication recommendations. It is crucial to develop explicit guidelines regarding the timing and manner in which patients are informed about the involvement of AI in their treatment, clinical trials, or diagnostic processes to foster transparency and build trust.

Another barrier is regulatory compliance, as AI technology must adhere to stringent pharmaceutical norms and standards, demanding validation for clinical use and navigating complex regulatory procedures. Ethical dilemmas also emerge, especially concerning data privacy, informed consent, and the potential for AI misuse. It is imperative to establish clear guidelines and consent procedures to guarantee the ethical deployment of AI[35].

Regulatory bodies such as the FDA and EMA are striving to impose strict regulations on the use of AI in drug development, which includes data management, model validation, and monitoring real-world applications. Collaboration among regulators, industry leaders, and scientists is essential to ensure that AI-driven innovations adhere to safety, efficacy, and ethical standards.

Intellectual Property Rights

Another concern is intellectual property rights, which make it difficult to determine who owns AI-generated findings. The quality and reliability of data are critical for AI accuracy, yet acquiring and keeping high-quality datasets is difficult in pharmaceutical sciences. Furthermore, the high expense of incorporating AI technologies may limit accessibility, especially in low-resource settings, potentially exacerbating global healthcare disparities. Overall, while AI has the potential to revolutionize pharmaceutical sciences, it is critical to address these obstacles and ethical concerns in order to ensure that the advantages are achieved ethically and equitably.

FUTURE PERSEPECTIVES

1. Continued advancements in AI technology and improved collaboration between pharmaceutical experts and AI researchers are expected to significantly boost the effectiveness and success rates of drug development processes[1] .
2. To fully realize AI's promise to transform drug development and, eventually, enhance patient outcomes, it will be imperative to address current limitations and ethical dilemmas as the field develops.
3. Regulatory bodies like the FDA and EMA are striving to impose strict regulations on the use of AI in drug development, which includes data management, model validation, and monitoring real-world applications. Collaboration among regulators, industry leaders, and scientists is essential to ensure that AI-driven innovations adhere to safety, efficacy, and ethical standards .

4. The high expense associated with AI infrastructure could restrict access, particularly in countries with limited resources. In order to guarantee fair access to the advantages of AI-enabled medication research and development, it will be crucial to address this dilemma.

CONCLUSION

Artificial intelligence (AI) is transforming drug discovery and development, providing unprecedented opportunity to speed and optimize the entire process from bench to bedside. Using machine learning, deep learning, and natural language processing, artificial intelligence is transforming drug development at multiple stages, including target selection, compound screening, lead optimization, and clinical trial design. High success rates in drug discovery and notable savings in time, money, and labor have resulted from the incorporation of AI [14] [11] .

AI's impact is evident across multiple areas, including virtual screening, toxicity prediction, and personalized medicine approaches. It has enabled more efficient analysis of large datasets, improved prediction of drug efficacy and safety, and facilitated the design of adaptive clinical trials. AI-designed compounds like EXS-21546, which have successfully entered clinical trials, show how this technology can shorten the time it takes to develop new drugs[4] [6] [14] [12] [11] .

However, implementing AI in drug research and development presents obstacles. These include the need for high-quality data, issues with model interpretability, regulatory hurdles, and the requirement for specialized expertise. Ethical concerns about data privacy and potential biases in AI systems must also be addressed. Additionally, the high costs associated with AI infrastructure may limit accessibility, particularly in resource-constrained settings.

Despite these limitations, artificial intelligence appears to have a bright future in drug development and discovery. Ongoing advancements in AI technology and improved collaboration between pharmaceutical experts and AI researchers are expected to significantly boost the effectiveness and success rates of drug development processes. As the area develops, it will be essential to resolve existing constraints and moral conundrums to realize AI's full potential to transform medication research and, eventually, enhance patient outcomes.

Authors Contribution :

Abou Taher: Conceptualized the study. Mohamed Ameen & Akash M V: Conducted the investigation. Mrs. Jiji K: Supervised the Manuscript preparation. Yaswanth Keerthi: Drafted the original manuscript. Gowtami V: Reviewed and edited the manuscript. All authors reviewed and approved the final manuscript.

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HOW TO CITE: Jiji K, Abou Taher, Akash M. V., Gowtami V, Mohamed Ameen, Yashwanth Keerthi, From Bench to Bedside: How Artificial Intelligence is Reshaping Drug Discovery and Clinical Trials, Int. J. of Pharm. Sci., 2025, Vol 3, Issue 8, 3159-3171. https://doi.org/10.5281/zenodo.17008073