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IP International Journal of Comprehensive and Advanced Pharmacology

Journal homepage: www.ijcap.in

Short Communication

Contribution of artificial intelligence in pharmaceutical drug discovery

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Abstract

Every aspect of science has been impacted by the development of computing and technology. One fundamental area of computer science that has influenced every field of research and technology, from basic engineering to medical, is artificial intelligence. Artificial intelligence is being widely employed to enhance medication design methods and time requirements. This method also makes it easy to identify the target proteins, increasing the likelihood that the therapies will be successful. Every stage of the medication design process makes use of artificial intelligence technology, which significantly lowers costs and lessens the health risks associated with preclinical studies.

Keywords: Data mining, Artificial intelligence, Pharmaceutical science, Medication creation, Healthcare.

Received: 23-02-2025; **Accepted:** 28-03-2025; **Available Online**: 07-04-2025

1. Introduction

Artificial intelligence has become a potent instrument that uses human knowledge to solve complicated problems quickly. Significant developments in machine learning and artificial intelligence technologies provide a game-changing prospect for pharmaceutical dosage form testing, formulation, and drug discovery. Researchers may find disease-associated targets and forecast how they will interact with possible treatment options by using algorithms powered by machine learning that analyse vast amounts of biological data, such as proteomics and genomics. This increases the possibility of successful medication approvals by enabling a more focused and effective approach to drug research. Additionally, streamlining research and development procedures can help lower development expenses. In addition to predicting the pharmacokinetics and toxicity of potential drugs, machine learning techniques aid in designing experiments. By prioritizing and optimizing lead compounds, this capacity lessens the need for expensive and time-consuming animal testing. Artificial intelligence algorithms that analyse real-world patient data can support personalized medicine methods, improving patient adherence and treatment results.

The healthcare sector is one prominent industry that is vital to saving lives. To solve global healthcare concerns and responding to medical catastrophes, like the previous pandemic, it is predicated on ongoing innovation and the adoption of novel technologies.[1] Innovation in the healthcare industry is usually based on a great deal of research and development in several areas, such as manufacturing processes, packing factors and customer-oriented advertising strategies.[2] The process of finding and creating new drugs, or drug discovery, is a difficult and drawn-out undertaking that has historically relied on labour-intensive methods like high-throughput screening and trial-and-error research. However, by facilitating more accurate and effective analysis of vast volumes of data, artificial intelligence techniques like machine learning and natural language processing provide the potential to speed up and enhance this process.[3] The authors of[4] recently reported on the effective application of deep learning to accurately forecast the efficacy of medicinal molecules. The toxicity of potential medications has also been predicted by artificial intelligence-based techniques. These and other studies have demonstrated AI's potential to increase the efficacy and efficiency of drug development procedures. But there are drawbacks and restrictions to using artificial intelligence to create novel bioactive substances. To

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https://doi.org/10.18231/j.ijcaap.2025.009

completely comprehend the benefits and limits of AI in this field, further study is required, and ethical issues must be considered.[6] Notwithstanding these obstacles, it is anticipated that AI will play a major role in the creation of novel drugs and treatments during the next years.

2. Discussion

Developing medication molecules with the best possible advantages and appropriateness for use in the healthcare sector is one of the main goals of the pharmaceutical business. Despite this, the pharmacy sector still must overcome several challenges that call for more development through technology-driven approaches to meet global medical and healthcare needs.[7] AI is a powerful tool for data mining based on machine learning and vast amounts of pharmaceutical data. Therefore, de novo drug design, activity scoring, virtual screening, and in silico evaluation of a drug molecule's characteristics including absorption, distribution, metabolism, excretion, and toxicity, have all made use of artificial intelligence.

In many respects, drug research and discovery has been transformed by artificial intelligence. Target discovery, virtual screening, structure-activity relationship modelling, de novo drug design, drug candidate optimization, drug repurposing, toxicity prediction, and more are some of the major contributions of AI in this field. The rate of penetration depending on the route of administration is one of the most important parameters for effective drug delivery system monitoring. The medication must pass through the intestinal or gastric epithelium after entering the stomach environment. The drug's continued distribution into the circulation depends on this phase. The medicine is delivered to the target site, which may be tissue or any cellular component, during the distribution stage.[8] Drugs may potentially enter the body through intracellular molecules. AI has the advantage of gathering data from many sources and indicating how the chosen medication delivery method should function to provide the desired outcomes. The assessment of patient, pharmacokinetic, and molecular data is regarded as a component of the complicated data for analysis to potentially choose the most effective active pharmaceutical to treat patient conditions or needs. To identify molecular entity properties and compare them to those of known compounds, the passive kind of artificial intelligence model is used. The precision of the medication delivery system selection, which artificial intelligence provides, is essential to effective therapy.

Computational pharmaceutics, which uses multiscale modelling techniques to improve medication delivery systems, is a result of the pharmaceutics industry's combination of artificial intelligence and big data. AI algorithms and machine learning techniques are used in computational pharmaceutics to analyse big datasets and forecast medication behaviour. By modelling medication formulation and delivery processes, researchers may evaluate various scenarios and optimize drug delivery systems without requiring a significant amount of trial-and-error testing. This reduces costs, increases productivity, and shortens the time required to develop new medications. Computational pharmaceutics models drug delivery systems at several scales, from micro to macro level behaviour. To forecast drug behaviour at every scale, the AI model algorithms can analyse intricate correlations between pharmacological qualities, formulation ingredients, and physiological parameters. This facilitates the development of effective drug delivery devices and enables a more thorough knowledge of drug delivery processes. It aids in forecasting the medication's stability, in vitro drug release profile, and physicochemical characteristics.

Drug discovery, preclinical research, clinical trials, and regulatory approval are all steps in the intricate process of developing new drugs. Because they establish the ideal dose, mode of administration, and safety of a medicine in the body, thus, pharmacokinetics and pharmacodynamics are essential components of drug discovery and development.[9] Studies on pharmacokinetics and pharmacodynamics have historically been carried out using experimental techniques including animal research and human clinical trials can be costly and time-consuming, and they might not always yield reliable forecasts of a drug's safety and efficacy.[10]

In the domains of drug development, pharmacokinetics, and pharmacodynamics, artificial intelligence has demonstrated enormous promise.[11] The method has become a useful tool for forecasting and improving medication pharmacokinetics and pharmacodynamics with the development of sophisticated computing and machine learning techniques. AI has the potential to expand the field of pharmacokinetics and pharmacodynamics research and its influence on treatment, despite the difficulties associated with massive data and trustworthy datasets.[12,13]

The drawbacks while depending on the artificial intelligence tools' may include the requirement for huge datasets, possible biases, and interpretability issues, notwithstanding their advantages. Therefore, to guarantee the safety and effectiveness of medications, AI-based models have to be employed in conjunction with conventional experimental techniques. The inability to integrate fresh data, biases in data, lack of transparency in AI-based drug development tools, limited capacity to account for variability, restricted data availability, interpretation of results, and other ethical issues are some of the potential drawbacks.

3. Conclusion

In summary, the drug discovery process might undergo a revolution thanks to artificial intelligence, which could speed up drug development, increase efficiency and accuracy, and enable the creation of more individualized and effective medicines. However, the availability of high-quality data, the resolution of ethical issues, and the understanding of the

limits of AI-based methods are necessary for the effective use of AI in drug development. With its application in pharmaceutical and biomedical research that is essential to the socioeconomic advancement of the common people, artificial intelligence can even have a remarkable impact on the healthcare industry. Of these studies, we can highlight those that have been carried out with the aim of treating diseases like cancer and neurodegenerative diseases, among others. In parallel, the lengthy medication development process necessitates the use of artificial intelligence to speed up medical research.

Promising approaches to overcoming the difficulties and constraints of artificial intelligence in the context of drug discovery are provided by recent advancements in the field, such as the application of data augmentation, explainable artificial intelligence, and the integration of artificial intelligence with conventional experimental techniques. The potential advantages of artificial intelligence, along with the increasing interest and attention from researchers, pharmaceutical firms, and regulatory bodies, make this a fascinating and intriguing field of study that might revolutionize the drug discovery process.

4. Source of Funding

None.

5. Conflict of Interest

None.

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Cite this article: Dubey S. Contribution of artificial intelligence in pharmaceutical drug discovery. *IP Int J Compr Adv Pharmacol*. 2025;10(1):69–71.