ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND PREDICTIVE HEALTH: A REVIEW

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Abstract
Artificial Intelligence transforms the drug discovery (pharmaceutical) industry by exploiting huge data sets and computation capabilities. Advanced algorithms improve efficiency, accuracy and success rates in developing new therapy by reducing human workload, cost and time. AI is also used in personalised medicine and new therapies to match patient needs. The use of AI aids for diagnosis and treatment increases during COVID 19 pandemic. AI predictive capability enhances clinical trial's reliability. It also optimizes treatment strategies and improves healthcare access.
Keywords: *Artificial Intelligence, Drug Discovery, Machine Learning, Deep Learning.*

Introduction:

Artificial Intelligence drastically changed many industries like manufacturing, agriculture, automobile industry, voice recognition, healthcare and medical diagnosis [Chen Fu et.al 2025].

AI transform healthcare and pharmaceutical industry for disease diagnosis, medical treatment and disease prevention. AI driven drug discovery enabled personalised treatment based on individual factors like drug design and new therapy drug development, [Oladele Oluwaseyi Kolawole 2024]. Drug discovery process involves target identification, compound discovery, optimization for enhancing health. It improves clinical trials efficiency by refining patient selection and monitoring treatment. [M. K. G. Abbas et al 2024].

Traditional drug delivery systems safely and effectively deliver therapeutics. This method has limitation related to proteins and nucleic acids [Mitali Panchpuri et al 2025].

AI helps speed up drug discovery, improve clinical trials and personalize treatments. Data collection and cleaning are essential in ML as the quality of the model relies on data quality. It is important to check and fix noise, biases and variance [Dolores R. Serrano et. al 2024].

AI can analyse large amounts of patient's data, helping doctors to choose the best treatment and monitor health closely. It also predicts disease and treatment outcomes [Yosri A. Fahim et al 2025].

AI plays an important role in healthcare and pharmaceuticals, addressing key challenges in drug discovery and development. Traditional methods face significant bottleneck such as target identification, high throughput screening and costly optimization process, which hamper efficiency and timely delivery of treatments. [Shashi Kant et. al 2025].

This paper discusses how AI can change drug discovery and development by making process more efficient and accurate. It also presents successful case studies to guide improvements in drug discovery for better healthcare [Maria Kokudeva et. al 2024].

This review paper explores the impact of AI on personalised medicine and drug discovery. Its aim is to analyze role of AI in drug development, examine its effectiveness in treatment and evaluate future trends in healthcare innovation. This paper discusses AI impact on diagnostics and equity through affordable solutions.

Current challenges and limitations:

- Data availability
- Transparency
- Ethical concerns
- Privacy and ethical issues
- Accountability
- Reliability
- Risk Assessment

Overview of AI Tools

Machine Learning: ML is a part of AI that helps to create model to make predictions or decisions [Mitali Panchpuri et al 2025].

ML algorithms are important in drug discovery and can be divided into supervised and unsupervised types. Supervised learning predicts how effective drugs will be using data from known compounds while unsupervised learning finds patterns in unlabelled data [Shashi Kant et. al 2025].

Deep Learning: DL is a powerful tool for modelling. It offers the potential to revolutionize the medical image and data analysis for research and disease diagnosis [Mitali Panchpuri et al 2025].

Natural Language Processing: NLP is a branch of AI its goal is to understand and interpret human languages. It can be particularly useful in personalised medicine. NLP is also used in pathology [Mitali Panchpuri et al 2025].

Neural Network: NN are crucial in AI, consisting of numerous neurons like units that generate output through functions. These models can model complex patterns with arbitrary complexity [Mitali Panchpuri et al 2025].

Disease Diagnosis:

Disease diagnosis is about finding the cause of a patient's symptoms. AI is changing this field by helping doctors with early detection of condition. This is especially useful when traditional methods fail. AI is used to predict various sever diseases. ML is advancing heart diagnosis with deep convolutional NN to detect irregular sounds. AI and ML are improving accuracy and speed in diagnosing various health conditions [Pranay Kurariya et al 2023].

Drug Discovery:

Drug discovery is a complex, multistage process for finding new medications which involves identifies potential drug candidates that can treat a disease. It integrates biology, chemistry, computational science and clinical research.

AI applications in drug discovery:
1. AI in drug target prediction
- Analyses biological data effectively
2. Machine learning applications
- Predict disease risk
3. AI in drug discovery
- Reduces costs in drug development
4. Drug optimization
- Analyses datasets to predict solubility, stability and utilizes databases for efficient drug design
5. Predictive modelling
- Reduces risks and improves drug candidate prioritization [Shashi Kant et. al 2025].

The comprehensive integration of AI in drug development increases efficiency and overall success rates in bringing new therapies to market. This innovation contributes more systematic and effective drug discovery process.

AI in real world applications:

AI has changed drug discovery by improving drug design, optimizing molecular properties and expanding its libraries. Atomise and BenevolentAI platform use AI to analyze data, discover and design new drugs, achieving success in finding compounds for disease like Ebola and COVID 19.

AI also aids in drug recycling by quickly analysing data to find new uses for existing drugs. In clinical trials, AI enhances designs, speeds up patient recruitment, allows real time monitoring [Shashi Kant et. al 2025].

Success Stories in Drug Discovery:

In 2024, DeepMind and Isomorphic Labs launched AlphaFold 3, an advanced AI system that significantly enhances the accuracy of biomolecular modelling. This tool predicts protein interactions with various molecules, including DNA and small compounds with greater accuracy. This model presents substantial advancement for researcher, facilitating a deeper understanding of disease mechanisms and creating new opportunities for drug discovery.

Insilico medicine are leveraging generative AI to develop innovative cancer therapies. This demonstrates significant anti tumour efficiency and safety, understanding the potential of AI in revolutionizing drug design and development processes. Overall, AI integration into drug discovery marks a transformative shift in the biomedical field, promoting innovation and efficiency.

Benefits of AI in drug discovery

AI is revolutionizing drug discovery by enhancing patient stratification, optimizing treatment strategies and development of new medications. AI enables healthcare provides tailor treatment more effectively by identifying distinct patient groups based on disease profiles. This personalized approach combined with advanced predictive modelling and biomarker identification, increases the success rates of drug development and ultimately improves the patient outcomes.

AI can predict the interactions and optimal dosages of multiple drugs for complex diseases. The integration of AI in drug development accelerates the identification of potential drug targets through rapid analysis of large datasets, facilitating quicker lead discovery and significant saving in time and resources for pharmaceutical companies.

Current and future perspectives of AI:

AI and ML are improving areas like radiology and treatment decisions, with advancements in drug compliance and medical imaging interpretation. The rise of AI concerns about how doctor patient relationship might change [Pranay Kurariya et al 2023].

Conclusion:

The pharmaceutical industry is changing significantly as Artificial Intelligence is being integrated into drug development. This combination of human knowledge and AI technology can

improve drug discovery, make research faster and create better treatment. As the industry collects more data role of AI is growing in healthcare sector AI will be vital in enhancing pharmacovigilance, allowing quicker identification of safety problems and better patient care. As used of AI in drug discovery increases it can lead to safer and more personalized treatments, transforming healthcare.

AI algorithms are effective in drug discovery and predictive analysis. They can analyse complex data and make predictions. Wearable technologies can improve personalized medicine by monitoring health indicators in real time, offering accessible innovations. Collaboration between AI researchers and clinicians is essential for effective AI use in clinical settings, with an emphasis on clear communication and standardization.

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