



Artificial Intelligence in Drug Development - Revolutionizing Drug Discovery and Clinical Trials

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Abstract

The integration of artificial intelligence (AI) in various spheres has revolutionized industries, and its impact on pharmacological science and medical research stands particularly profound. With AI's multidisciplinary applications, especially in drug development and clinical trials, this technology emerges as a pivotal tool to streamline the lengthy and costly process of traditional drug discovery.

In the medical realm, AI algorithms are deployed for disease detection, medical imaging, clinical trial efficiency, and patient outcome predictions. Post-COVID, the surge in AI research underscores its relevance and potential in shaping the future of healthcare. However, challenges arise in accessing electronic medical records (EMRs) due to confidentiality regulations, hindering seamless data acquisition for AI-driven analyses.

Despite its transformative potential, the application of AI in drug discovery and clinical trials faces hurdles concerning regulatory compliance and participant privacy. Addressing these challenges necessitates transparent AI mechanisms, fostering regulatory approval and instilling participant confidence in studies.

In conclusion, while AI's integration in drug discovery promises enhanced efficacy and reduced complications in clinical trials, navigating legal obligations and ensuring transparent AI systems are pivotal for its sustainable implementation. As AI continues to evolve, its trajectory augurs well for resource optimization and minimized complexities in drug development and clinical trials.

Keywords: Artificial Intelligence; Pk-pd Studies; Electronic Medical Records; Data Analyses; Technology

Introduction

Artificial intelligence (AI) is a mechanical or digital simulation of human mind where the software or instrument can plan and predict the outcome [1]. In simple words they consist of 3 layers, perception, cognition and decision making. Combining with data storage, machine learning (ML) and AI framework development it has now widely integrated with cyberspace, basic experimental science and has hugely affected human life [2]. In the field of pharmacological science and research drug development is an important and lengthy process that requires lots of patience and fund-

ing. The conventional way takes around 10 - 12 years, and cost may reach up to USD 1 billion [3]. Reason behind this is the complex and unknown physiology and functional mechanism involved in receptor level or hormonal, physiological and neurohormonal status [4]. The cost and the time requirement can be reduced by focusing in designing a molecule at its specific working level at highest precision and the probable toxicity and other pharmacokinetic properties also can be predicted by considering tissue selectivity, SAR, potency, and required dose for optimizing drug efficacy [5]. So precision in molecule designing is a necessity of today.

AI in present day

Application based on artificial intelligence (AI) has emerged as a multidisciplinary dimension, starting from sports, educational activity, IT sector, as well as in the advancement of various scientific research works. AI algorithms are becoming popular now a days in decision making for patient outcome in the form of disease detection, medical imaging, clinical trial efficiency, drug development etc. [6]. Research works on AI has tremendously increased particularly in post covid era denoting its importance [7].

AI in pharmacology and medical world

Like in all other fields the use of AI technology has grown up with huge popularity in pharmaceutical research. Various algorithms gained from the real world data gathered from multiple geographical regions are being used to predict the pk-pd behaviour of the compound, its characteristics, pharmacogenomics profile and these data are widely used for the initial designing of the drug molecule [7].

The process through which AI works in medical science is known as machine learning (ML). This technology mainly predicts the outcome depending on the analysis of different data based on statistical recording. The basic of both AI and ML lies upon two arms. In one side there is a theoretical model, where the experimental model learns upon training resulting into interpretation of the data store and evaluation of the data [8].

Utility in drug discovery

Conventionally drug discovery consist of broadly preclinical and clinical studies. The assessment of drug toxicity, Pk-Pd profile, and various *in vitro* methods are also included there. Any developmental process starts with many lead compounds, but at each stage one or few are excluded and ultimately one compound remains for marketing approval [9]. Each phase in clinical trial takes long duration, 7 - 8 months in phase I up to 4 - 5 years in phase II and III. Also extra time is needed for patient recruitment, documentations and legal formalities. There is around 32% failure rate in various trial because of faulty recruitment technique has been observed in different reports. Systems comprising with AI and ML can assist improvising patient selection and cohort composition [10]. Apart from this, different AI techniques like deep learning (DI), natural language process (NLP), optical character reasoning (OCR), human machine interface (HMI) can be applied to modify

and compile the data from electronic storages (Databases) of diverse areas to be analysed.

Complications of data gathering

The main problem occurs during an AI assisted study is accessing the electronic medical records (EMR) is the confidentiality as most the medical data are kept secured by different authorities or institutions because of legal obligations, known as EMR interoperability dilemma which require substantial investment by government and medical institutes [11], whereas legal authorities like US Health Insurance Portability and Accountability Act (HIPAA) and the EU General Data Protection Regulation (GDPR) protects the third party accession of sensitive clinical data which impacts ML and DL systems to gather required statistical information [12].

Conclusion

Different AI methods can be broadly applied to drug discovery process. These are helpful in reducing trial complications and improvement in study outcome. But its application doesn't come without drawbacks. The most important complication occurs in the form of legal obligations. To overcome this easy explainability of AI system and mechanism is important to avail regulatory approval, and to secure participants confidence in the study. AI technology is now becoming very popular these days and with further development the utility will be obviously help in saving resource and manpower with less complications in clinical trial and simultaneous drug discovery.

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