

“Artificial intelligence in drug discovery and development”

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Abstract:

Artificial intelligence (AI) is remodeling drug discovery and development field by enhancing the efficiency, accuracy and reducing the cost and time. Traditional drug discovery is costly and time consuming process involving target identification, lead optimization, preclinical and clinical studies. By using the deep learning, machine learning and reinforcement learning to quickly analyze the vast biomedical datasets, researchers can efficiently predict drug target interaction and develop therapeutic molecule. Additionally, AI improve the drug development by enhancing clinical trials design, improving patients selection, support personalized medicine approaches and predicting adverse drug reaction. AI advantages and challenges includes the data quality, regulatory concern, model interpretability.

Key words: Artificial intelligence, Drug discovery, Drug development, Clinical trial, Deep learning, Machine learning.

Introduction

The traditional drug discovery and development is very complex process requires 10 to 15 years form lead identification to product development. It is very complex and challenging process takes \$1 to 2 billion for each marketed approved drug and requires lot of clinical and preclinical data.[1] The lower effectiveness and high cost of traditional method of drug development is very challenging therefore it is need to develop new methods to avoid time consuming and increasing cost of conventional methods of drug development. [2] In 2020 the COVID -19 pandemic situation in world wide highlighted the need of new techniques of drug discovery and development for better effective treatment.[3] Artificial intelligence (AI) has grows as an important in drug design due to its ability to process large amount of datasets, it offered accuracy, high speed and effective tool for drug discovery process.[4,5]

Scope and objectives

- 1)Procurng integrating biological data including (electronic records of health, screening). [6]
- 2)Artificial intelligence (AI) carried out interpreting processing of scientific literature, help researchers to uncover difficult therapeutic target. [4]
- 3)It accelerated drug development process by avoiding conventional trial and error process of drug development.
- 4)It helps in predicting toxicity and ADME profile of drug candidate an enabling more effective and accurate analysis of data.[5]
- 5)In clinical practices AI supports in laboratory diagnosis, in clinical decision making, personalized medication, pharmacovigilance. [6]

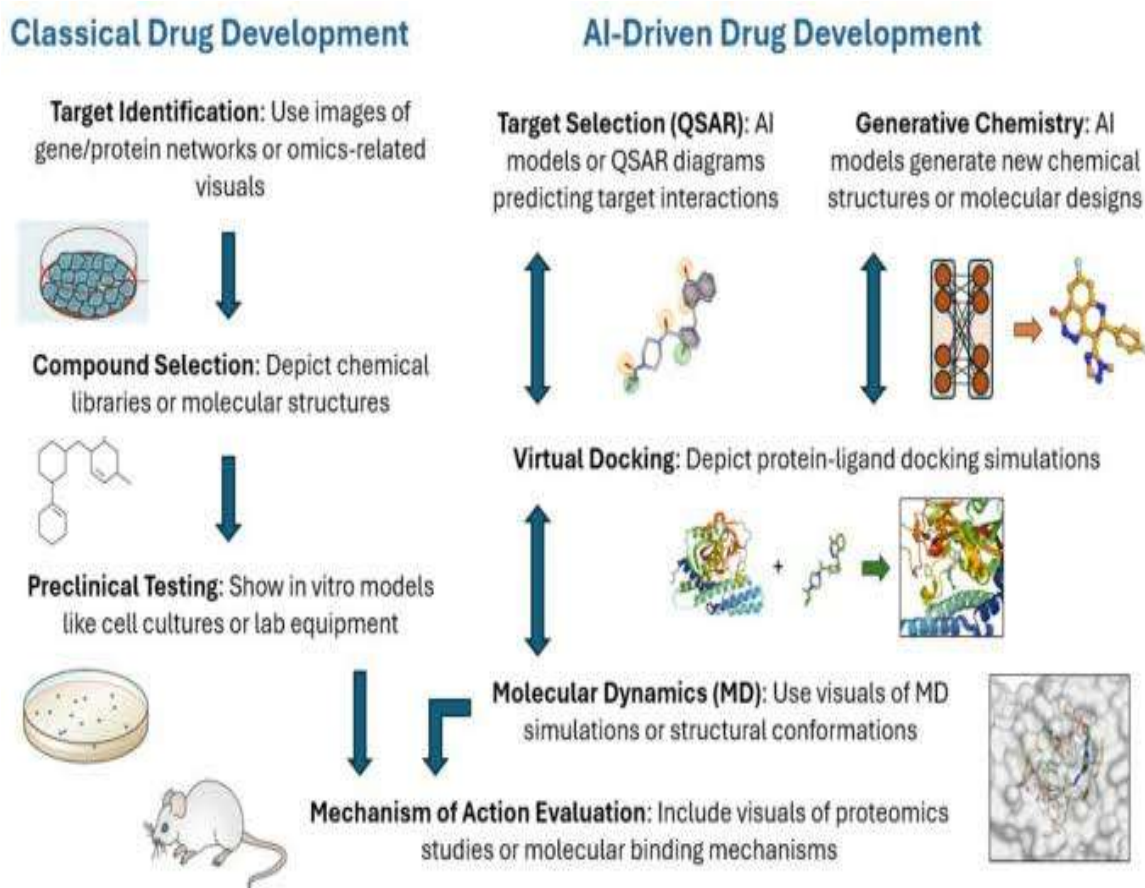
Artificial intelligence (AI) in Drug Discovery

There are large number of chemical compounds the absence of novel technology causes lengthy and costly process in drug development use of AI mitigated this problem.AI driven techniques like machine learning, deep learning and reinforcement learning produces new drug candidate. [4,6]

Artificial intelligence is a widely growing field in lead identification this enhance the efficiency and accuracy of new candidate development. Nowadays AI has been used in several stages of candidate drug molecule identification including molecular target identification, drug screening, lead compound optimization, pharmacokinetics study and toxicity prediction. [7]

Despite it's all important in drug discovery and in drug development AI faces many critical challenges of scale, diversity of data. AI helps in quantitative structure activity relationship which further large amount of log P parameters. [8] Drug discovery carried out when there is a sudden result occur due to outbreak of pandemic situation or when there is a no treatment available for diagnosis of disease, in case of treatment of rare disorder or when existing drug do not show optimum amount of efficacy. Drug discovery requires activation or inhibition of certain molecules of body e.g. enzyme which play role in wellbeing. [9]

Two types of AI application in medicinal field i.e physical and virtual. Robot assisted surgery, real time patient monitoring, automated laboratory processes and AI enhance prosthetics those are involved in the physical application in the medicinal field. For e.g., robot assisted surgery in AI can give the medical professional along with necessary related information to help them in making many clear decisions those AI can't replaced healthcare professional it can help to improve patient care and improves the capability of medical professional due to these robots minimize penetration and reduce the risk of severity and early recovery and better surgical outcomes [10]



Basics of artificial intelligence used in drug discovery

1. Machine Learning -

Docking stimulation is frequently used for DTI prediction during the DDD process but is less appropriate for large scale for virtual screening because it is time consuming. Many machine learning techniques have been put forth to solve this problem by methodically searching the whole chemical universe for possible interaction with the target biological space.[11] Artificial intelligence based tools for identification, prediction for compound effectiveness, drug targeting, toxicity prediction is accelerated by machine learning method. It leads to rapid drug development through lead discovery by predicting pharmacokinetics and pharmacodynamics profile also the adverse effect studies. [12]

Biological macromolecules which are made up of small molecules like cells is modulating by the action of drug moiety. Machine learning techniques has ability to differentiate action of drug moiety from non drug moiety on the targets [13] Machine learning based model helps in identifying uncover pattern that are not identified by traditional system of drug development in addition they play role in identifying potential toxicity of the new chemical entity which helps in prediction in drug development phases. Large amount of datasets doesn't readily predicted by human so ML helps in identifying and analyzing large datasets.[14]

2. Deep Learning -

Deep learning is one of widely used method in drug development appliance from drug target interaction to drug – side effect prediction. This method can easily tackle the problem. Various Deep learning models have power to effectively resolved complex problem that are difficult to solve by conventional methods.

Deep learning techniques classify into :

- a. Classical neural network
- b. Convolution neural network
- c. Recurrent neural network
- d. Generative adversarial network
- e. Self-organising maps
- f. Boltzmann machines
- g. Autoencoders [15]

Deep learning is more advance than the machine learning which used combinatorial non linear model that indirectly gives features at various levels from the high dimensional. Recently deep learning methods is based on the neural network model which have the multiple layer structure design due to mimic the human brain and also learn from large data volume deep learning is very useful tool is vast variety difficult field like computational chemistry, high energy physics, computational biology and medical diagnostic where the expert knowledge is required. [16]

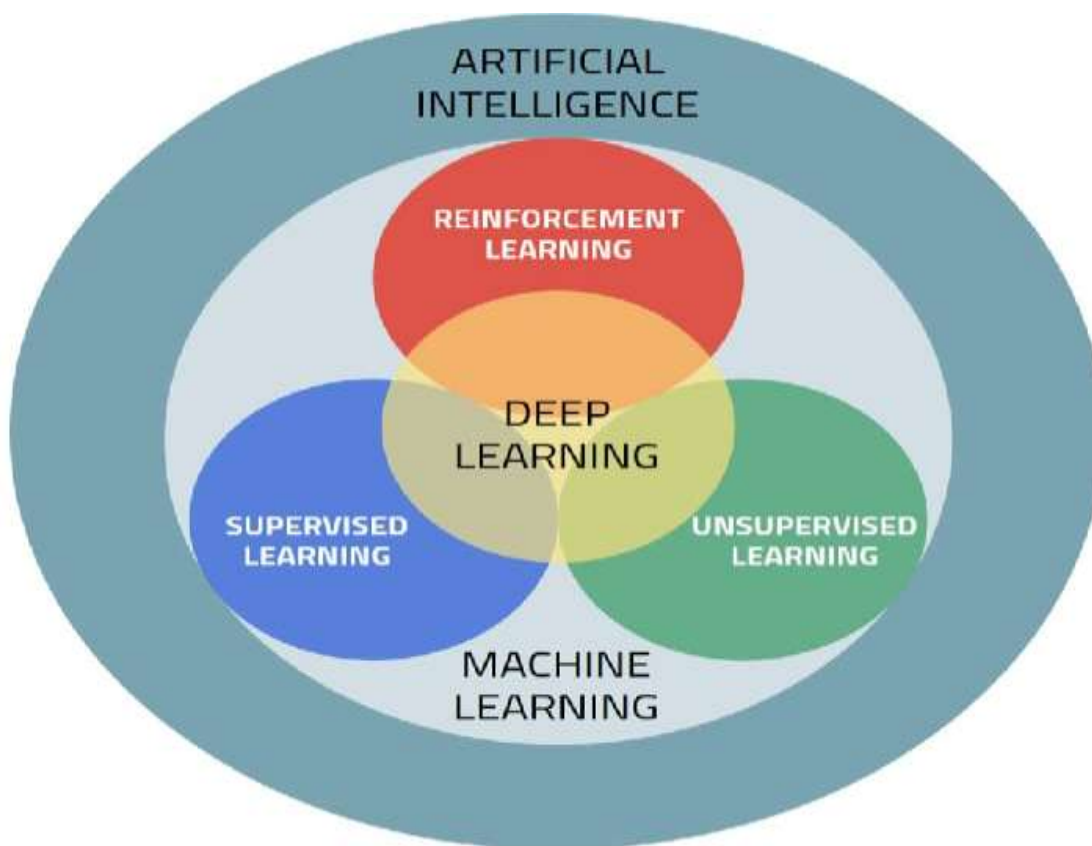
3. Reinforcement learning –

Reinforcement learning is used as substitute to guide the chemical space which fix goals and initiate actions in specific state due to increase the reward.

RL algorithm are classified as:

1. Value based (e.g. Q learning)
2. Policy based (e.g. policy gradient)
3. Hybrid (actor – critic) [9]

It is complex to regulate the properties of developed molecules using data driven presentation for e.g , developing a molecule with a particular set of physicochemical properties from large physicochemical search is delay and demanding in generative adverse aerial network RL is the machine learning that plays role in drug discovery process in the molecule genesis . [3]



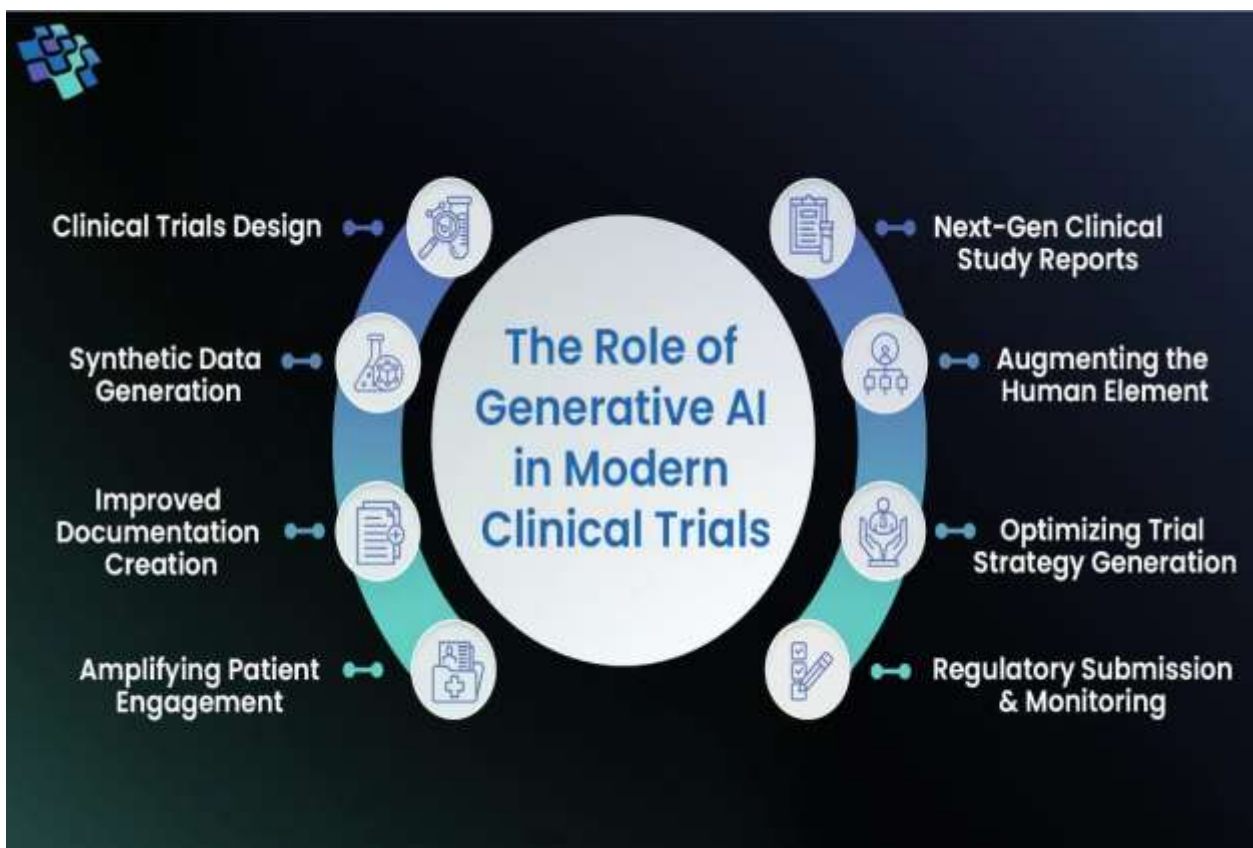
Clinical Trial

Analysis of Decentralized clinical trials, handling massive volumes of data are challenging task. For enhancing the data compilation AI & ML is very helpful. Before the medication is tested on humans, bio simulation—the process of simulating biological systems and processes on a computer using mathematical models—may be employed. These models helps in the investigation of topics like the best dosage, drug interactions, and efficacy for a large number of individuals.[6] Appropriate patient populations, improving trial outcomes and lowering recruitment failure is find by using predictive modelling and real word data analysis [4]

AiCure created mobile software that tracked patients with schizophrenia's regular medication administration in a Phase II trial. This enhancing patient adherence by 25%, guaranteeing the clinical trial's successful conclusion.[17] In order to improve patient matching for Phase I oncology clinical trials, researchers have created explainable AI techniques using natural language processing. This has improved drug development efficiency and addressed more patient recruitment challenges. These techniques use AI-driven tools to analyse patient records and complicated clinical trial eligibility requirements, ensuring that qualified candidates are found more quickly and accurately.[13]

AI tools are now widely useful in application of clinical trial design. Due to deficiency in preparation of drug, it cause the oncology and other diseases which decline the clinical trial failure rates. The high failure rates of drug production increase cost of drug development. Nowadays the use of AI clinical trial enhance organisation, efficiency, ultimately increases the success rate. AI software help to improve the success rate of clinical study in different complex areas like, medical literature, linking patient genetic data to conclude the toxicity ratio. Deep learning models help in determining efficacy, toxicity and potency. It helps in detecting phase 1 and 2 clinical trial. [16]

Before the marketing of new drug INDA this application is filled for approval of clinical trial. Clinical trial are arranged in different phases (Phase 1-5). In Phase 1 check the safety and efficacy of dose and there are 20-100 people healthy volunteer assess to it. Phase 2 check the effectiveness and adverse effects, it includes 100-300 sick patients. Phase 3 check the drawbacks of newly developed chemical entity in it includes 300-1000 patients. Phase 4 called as post marketing surveillance. [18]



Challenges

Some of AI tools like machine learning, deep learning, natural language processing, reinforcement learning are highly effective in drug discovery. [6] The overall success rate of artificial intelligence is dependent on significant amount of data provided is necessary for subsequent training program. Pharmaceutical industries can clarify that AI technology finding solution of complex problems also help to understanding the solution. [8]

In AI powered drug discovery a complex challenge is the availability of high-quality annotated dataset for the purpose of training the models. Data heterogeneity, in which data gathered from diverse sources, like chemical structure, biological assays and clinical trials, this poses a significant barrier. Incorporating and coordinating these disparate data sources into a unified format for AI training can be complicated and lengthy. Incorporation of AI in pharmacy practice brings significant improvement but also causes major ethical concern. A recent study conducted in the field of pharmacy in the Middle East and North Africa (MENA) region emphasizing a major problem such as cyber security threats (58.9%), patient data privacy (58.9%), potential job displacement (62.9%) and lack of legal regulation (67.0%). [19]

In AI discovery sometimes imperfect check against contextual understanding the current problem. This will help or support development of AI tool for drug discovery. In the AI development is refine the primary data before used for development. This data focus on quality of primary information about drug. Also it may be restock with help of AI tool. AI tool guide to prevent the harm happen in the development of drug, also give guideline about accountability, fairness for drug development and main focus on evaluation of drug. It helps to give quantify, measurement and a principle about the regulation of drug. Also guide about the drug promotion and share the process of drug development, gives the parameter of growth in the industry. It is venture or gain a future returns in education. [13]

The creation of ethical rule and management system and structure is essential to making accountable honest AI use guiding principle. This includes consideration such data security and approval. [14] Pharmaceutical company needs simplicity about the potential of technology decision making to problem once it's has been applied along with knowledge the reasonable goal that can be achieved. [17]

Application

Regulatory agencies are displaying improving benefits AIDD and its uses. The application of computational tools to measure carcinogenic potential of related adulterants has led to the addition of structure activity prediction as a part of regulatory filling. [19]

In the drug development the AI tools help to analysis in data discovery also help to predict the biological source or data base. The various book, novels, IP books, practical books, notes of AI technology are help in drug investigation. This help to increase in data development. AI tools called as drug bank. [12]

The field of AI in drug discovery is rapidly progressing research field, that use to improve efficiency and accuracy of the drug discovery process. AI play a significant role in drug discovery includes target identification, molecules screening and toxicity prediction. Noticeable ability of AI in drug discovery is to analyse and processes of biological records such as genomic study, proteomic and pharmacological data for the detection of potential drugs target. [20]

Conclusion

Artificial intelligence plays significantly important role in advancing discovery of new chemical entity and drug development. The recent basic of AI like machines learning, enhancing the clinical trials success rate. AI serve as a global platform for new research work. The reduction in expenses in research work and speeding the development process of new drug has become an urgency for both drug makers and for patient as well. Thus AI contribute as an essential tool for drug discovery and development.

References

1. https://www.researchgate.net/publication/380475067_Role_of_Artificial_Intelligence_in_Revolutionizing_Drug_Discovery?_tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Ii9kaXJlY3QiLCJwYWdlIjoicHVibGljYXRpb24iLCJwcmV2aW91c1BhZ2UiOiJfZGlyZWN0In19
2. <https://share.google/dYtVohXR6iyZuCEqn>
3. https://www.researchgate.net/publication/371884207_AI_in_Drug_Discovery_and_its_Clinical_Relevance?_tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Ii9kaXJlY3QiLCJwYWdlIjoicHVibGljYXRpb24iLCJwcmV2aW91c1BhZ2UiOiJfZGlyZWN0In19
4. https://www.researchgate.net/publication/400249756_Pharma_AI_Revolutionizing_Drug_Discovery_and_Healthcare_with_Artificial_Intelligence?_sg=0sIwrT-r1OpLh3tvgqc1Tq_ytZJ_Goz61wptB-PThZ-N5IDHpMmXDX2zEEgcpdyPoq0ZcKVyXecvU8c&_tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Ii9kaXJlY3QiLCJwYWdlIjoicHVibGljYXRpb24iLCJwcmV2aW91c1BhZ2UiOiJfZGlyZWN0In19
5. https://www.researchgate.net/publication/371713901_The_Role_of_AI_in_Drug_Discovery_Challenges_Opportunities_and_Strategies?_tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Ii9kaXJlY3QiLCJwYWdlIjoicHVibGljYXRpb24iLCJwcmV2aW91c1BhZ2UiOiJfZGlyZWN0In19
6. https://www.researchgate.net/publication/400249756_Pharma_AI_Revolutionizing_Drug_Discovery_and_Healthcare_with_Artificial_Intelligence?_sg=0sIwrT-r1OpLh3tvgqc1Tq_ytZJ_Goz61wptB-PThZ-N5IDHpMmXDX2zEEgcpdyPoq0ZcKVyXecvU8c&_tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Ii9kaXJlY3QiLCJwYWdlIjoicHVibGljYXRpb24iLCJwcmV2aW91c1BhZ2UiOiJfZGlyZWN0In19
7. <https://share.google/daNWRtoOzODk8H2mB>
8. <https://share.google/f49IX8j9wGazfwHKP>
9. <https://share.google/eNBjU1zsfS2Ids7HU>
10. <https://share.google/DRkKEyY9H7fFJmnxO>
11. <https://share.google/SFAyxp8tOcs0GUMZ2>
12. https://link.springer.com/article/10.1007/s44395-025-00007-3?utm_source=chatgpt.com
13. https://link.springer.com/article/10.1186/s40364-025-00758-2?utm_source=chatgpt.com
14. <https://www.frontiersin.org/journals/chemistry/articles/10.3389/fchem.2024.1408740/full>
15. https://www.researchgate.net/publication/365475348_Deep_learning_in_drug_discovery_an_integrative_review_and_future_challenges?_tp=eyJjb250ZXh0Ijp7ImZpcnN0UGFnZSI6Ii9kaXJlY3QiLCJwYWdlIjoicHVibGljYXRpb24iLCJwcmV2aW91c1BhZ2UiOiJfZGlyZWN0In19
16. <https://share.google/5DXOnHehbGbZumdGY>
17. <https://share.google/gDhFKIX2NkEay8Wpx>
18. https://www.researchgate.net/publication/397212689_Artificial_Clinic_Intelligence_ACI_A_Generative_AI-Powered_Modeling_Platform_to_Optimize_Patient_Cohort_Enrichment_and_Clinical_Trial_Optimization
19. <https://share.google/EAu5KhMca9rGn20ND>

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