Artificial Intelligence in Drug Development

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***Abstract*: Drug discovery is a complex process carried out by pharmacists carefully that can take up to years. Data in healthcare has become increasingly digitalized over time, particularly in the pharmaceutical industry. However, this presents numerous difficulties, such as acquiring, examining, and applying that knowledge to resolve clinical issues that can be excessively complex. Introduction of Artificial Intelligence has been proven to reduce the human workloads in this sector. Artificial intelligence refers to the processing of human intellect by machines, particularly computer systems. Medical chemistry has been applying AI in drug development since 1960s. Quantitative Structure-Activity Relationship (QSAR) approach is a prime example of this. QSAR is frequently used to forecast properties of chemical structures, including bioactivity and solubility, among others.**

***Keywords:* - Artificial intelligence, Drug development, Drug designing, pharmaceutical, Drug**

1. INTRODUCTION

Mechanical innovation is urgently needed in the pharmaceutical and drug industries to make it easier to produce drugs for human consumption. Because of the current resource constraints, developing and commercializing complicated processes drugs that are safe for human consumption and putting them into standard therapeutic usage has proven to be difficult. With the use of artificial intelligence (AI), computers may decide, carry out, and finish activities without human oversight or prior explicit programming. The ultimate goal of using AI is to deliver the best medications to the clinic in order to meet unmet medical needs. There are four ways that AI is currently applied in the pharmaceutical sector. The first is in determining the extent of a patient's illness and determining if the intended therapy will be effective for them even before it is administered. Second, it helps resolve and avoid treatment-related complications. Its third primary use is as a patient-assistive technology during medical procedures or operations. Lastly, it is used to determine the justification for using particular tools or substances during treatment as well as to invent or extrapolate new uses for those same tools or substances to improve their safety and efficacy. In the drug and development industries, AI-enabled technology is actively being adopted to address small but crucially important issues. The scope of AI applications for early drug discovery has significantly expanded. De novo drug design being an example. AI helps companies use vast sets of data to identify and develop a better drug.

2.DRUG DESIGNING

The process of developing new drugs or altering existing ones to treat diseases is known as drug designing. It involves the usage of computer models, simulations, and experiments to identify molecules that can interact with specific biological targets, such as enzymes or receptors, and exert a therapeutic effect. Which chemical structures will produce the desired property profile is one of the fundamental questions that can be asked in the drug development process. A computational model based on the quantitative structure-activity relationship (QSAR) can be used to quickly predict large numbers of compounds or simple physicochemical parameters, like log P or log D. The AI can aid in the design of drug molecules by foreseeing the structure of the target protein and the interactions between the drug and the protein. Since the design is in accordance with the chemical environment of the target protein site, AI can help in structure-based drug discovery by predicting the 3D protein structure. This would make it possible to foresee how a compound would impact a target. AlphaFold is an example for this. It predicts the 3D structure of the target protein by measuring the separation between nearby amino acids and the corresponding angles of the peptide bonds. The effectiveness of a therapy depends heavily on drug-protein interactions. The accuracy of ligandprotein interactions predicted by various AI techniques has improved therapeutic efficacy.

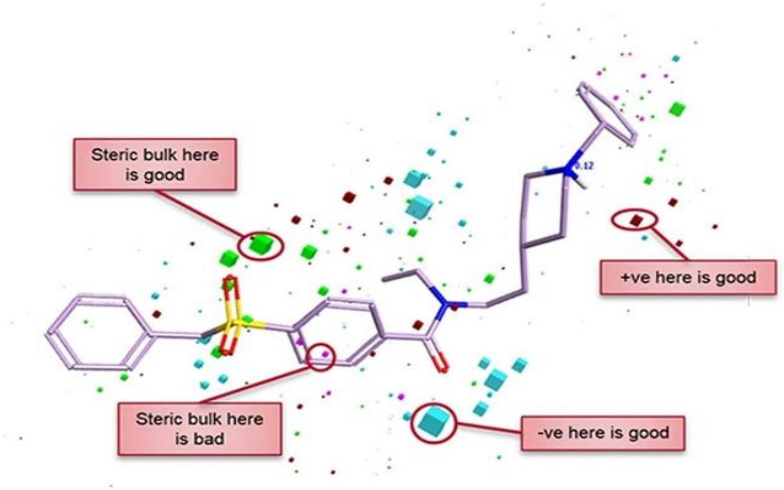

Fig. 1 QSAR Model of Artificial Intelligence in Drug designing

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3.DRUGSCREENING

Drug screening is the procedure which is used to identify and improve potential medications before choosing a candidate to move forward with clinical trials. It could have high-throughput screening assays that may be used in screen sizable chemical libraries for a specific biological activity, which could take a long time. By speeding up the identification of novel drugs and lowering the time and expense associated with drug development, artificial intelligence (AI) has the potential to completely transform drug screening. Machine learning algorithms, which can analyze large amounts of data from numerous sources, including genetic and molecular data, clinical trial results, and scientific literature, are one way AI is being used in drug screening. These algorithms can identify patterns and relationships that might otherwise be obscure to human researchers and can help to predict which drug candidates are most likely to be successful.

AI also uses virtual screening, where computer simulations are used to test the effectiveness of potential drugs.AI can also help clinical trials be more accurate by identifying the patients who will respond to a given drug the fastest.

4. DRUG REPURPOSING

Drug repurposing is the process of coming up with new applications for drugs that have already received human use approval. Artificial intelligence (AI) could have the potential to accelerate and enhance the drug repurposing process by identifying new therapeutic indications and potential drug combinations which might be ignored by humans. AI algorithms can screen databases of known drugs to find substances that have the potential to treat a particular disease or analyze gene expression data to identify potential drug targets for a particular disease. Large datasets of clinical trial data can be analyzed by AI algorithms to spot trends and forecast how various medications may behave in various patient populations. The protocols for drug dosing and treatment can be improved as a result, potentially identifying any safety issues. AI methodologies may be more useful in locating potential targets for repurposing.

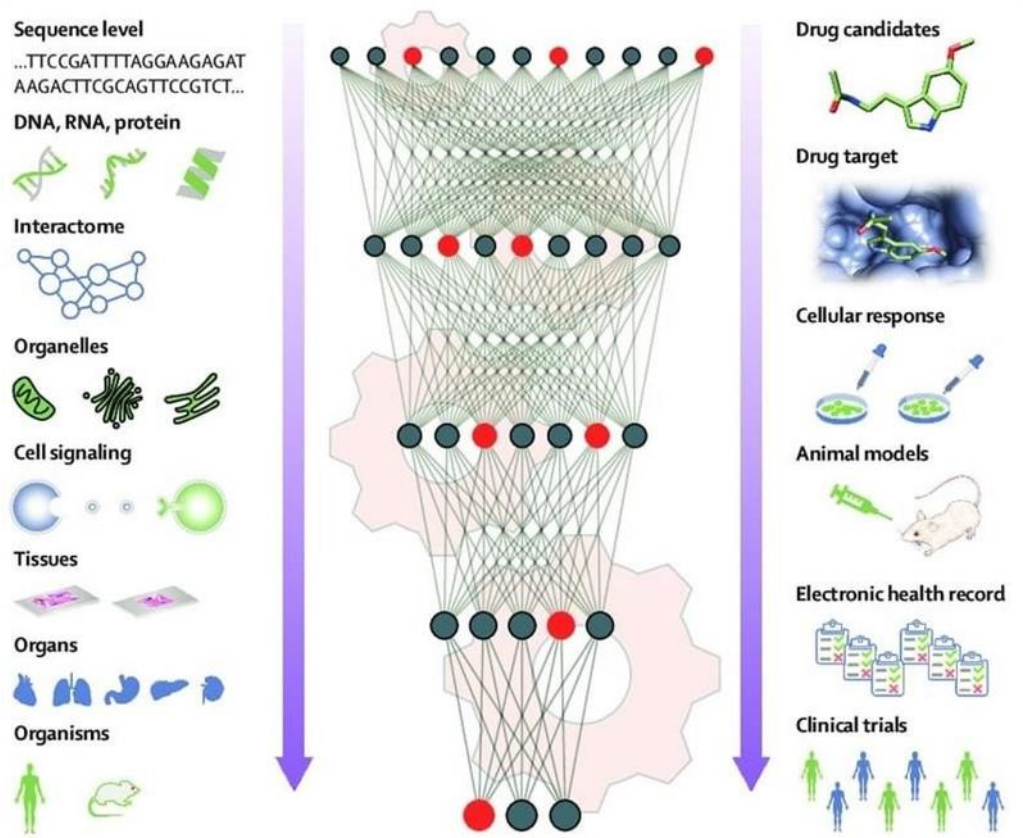

Fig 2. AI in Drug Repurposing

5.CHEMICAL SYNTHESIS

Chemical Synthesis is a process in drug development which deals with the preparation of a compound or molecule from available chemicals. Researchers frequently have to create new molecules from scratch in order to test experimentally whether they have the desired properties. If not, it would be necessary to create new molecules. This a tedious task. If researchers could accurately predict the characteristics of hypothetical molecules, they would be able to synthesize only the most promising molecules and avoid synthesizing and testing numerous molecules that do not have the desired properties. AI can be trained to identify stereochemical orientations during the reaction and forecast the viability of synthesis for a specific chemical reaction/compound. It is essential to develop the structure of molecules and predict their feasibility when developing a drug. Highly trained AI can considerably boost the development of new drugs with their structures and compositions, notably for the chemical synthesis of complicated natural chemicals. The AI platform can also be trained on a wide range of chemical reactions, which can ultimately provide more detailed and rapid insights into the chemical synthesis pathway and can deliver ideal reaction conditions that can optimize and deliver a better yield. For problems where the physical laws governing the predicted molecular properties are not precisely known, or when establishing empirical relationships would be too difficult, AI-based algorithms are particularly well-suited. As an example, consider the stacking method, in which AI can use the outcomes of predictions made by physical or empirical relationships as input data.

6.POLYPHARMACOLOGY

Polypharmacology involves how drug molecules interact with various targets to potentially disrupt one or more disease pathways. It is much more complex than targeting a single protein. It requires a better understanding of the structure activity relationship of the drugs. The amount of data that needs to be processed for drug development is enormous, and the current computational and to identify polypharmacological relationships between ligand binding to multiple targets, AI can find various similarity-based, network-based, and structural approaches. Drug discovery for conditions like cancer and diseases of the central nervous system is predicted to grow quickly with the use of AI for Polypharmacology modelling.

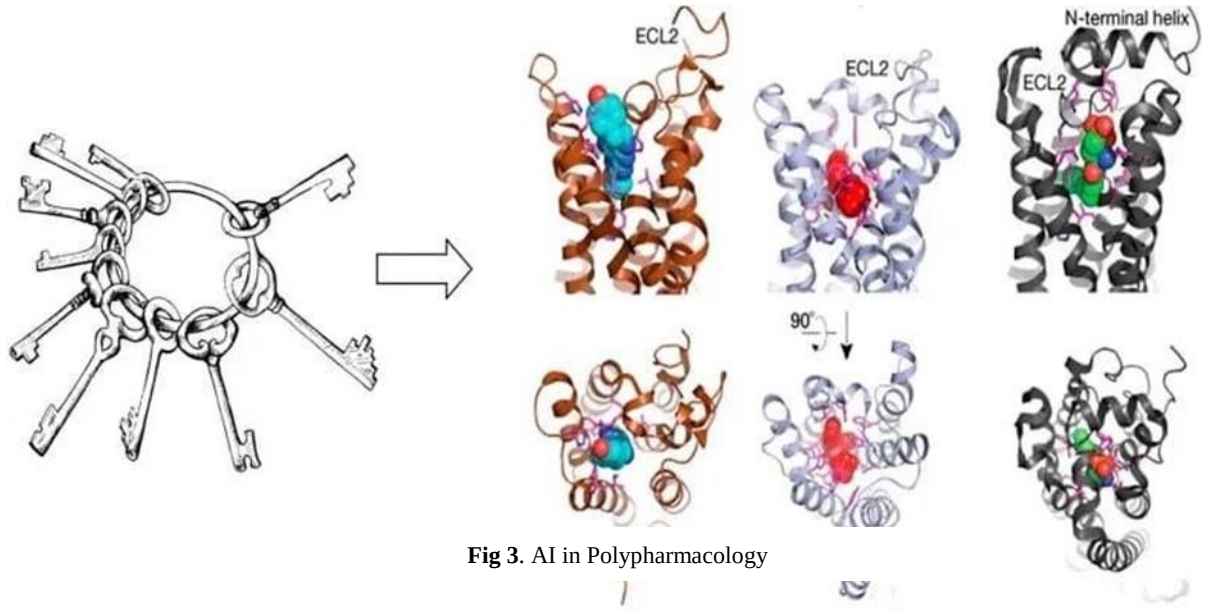

Fig 3. AI in Polypharmacology

7. CONCLUSION

Artificial intelligence is growing at an exponential rate in healthcare industry, especially in drug development. Artificial intelligence has a great deal of potential to change the process of discovering new drugs and developing them (AI). It can quicken the pace of drug development, identify new drug targets, and improve drug design. By anticipating patient response to treatments and optimizing dosages, AI can also help with personalized medicine. Drug design and development experimental and computational fields will continue to be early adopters of new and developing technologies. One of the challenges is using these technologies to enhance the current pipeline and processes. Big data, digital healthcare, remote monitoring, and genomics will be the driving forces behind the need to investigate how computational and reasoning approaches can be applied to enhance the process in terms of both clinical significance and cost reduction. The applications of artificial intelligence in healthcare are anticipated to expand thanks to the quick development of computer hardware, software, and mathematical models, which include a variety of techniques. In addition to drug development, the use of AI will in the upcoming years have a significant positive impact on fields that call for complex decision-making and critical thinking.

8.ACKNOWLEDGEMENT

We would like to sincerely thank and convey our gratitude to all the specialists and our mentor for their invaluable assistance and direction during our research.

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