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Popular Article

Application of Artificial Intelligence in drug discovery: A new paradigm in drug designing

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Introduction

AI is defined as the mimicking of human intelligence process by machines or making the machines to think like humans to perform tasks such as learning, problem solving, reasoning and identification of patterns. This involves collecting data, developing rules for utilizing the information, drawing definite conclusions and auto-correction. Now-a-days AI is used in every sector ranging from educational methods to business processes to achieve the definite goals with accuracy. Adoption of AI in the drug development process has turned it to hope. AI comes up with two sub-fields, machine learning and deep learning. Machine learning uses the statistical methods with the ability to learn with or without being accurately programmed. Deep learning comprises artificial neural networks that learn from the greater amount of experimental data.

Machine learning includes supervised, unsupervised and reinforcement learning. In supervised learning, one uses the classification and regression methods and based on the input and output sources predictive model is developed such as disease diagnosis, ADMET prediction and drug efficacy. Unsupervised learning is based on clustering and feature finding methods. This uses solely input data for grouping and interpretation and can be utilised for discovery of disease subtype and target. Reinforcement learning involves decision making and the execution of the performance of a given problem. It can be applied for experimental designs and de novo drug designing which uses of modelling and quantum chemistry. Deep learning has emerged rapidly due to vast amount of data and increasing growth of computer capacity. Exploring into vast data and algorithm methods can offer us new compounds that could be potentially new medicine,

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helps us to unveil the repurposing of drugs and personalized medicines. Drug discovery is a time taking, costly and laborious process. Establishment of AI in the methods of drug discovery will witness the minimum failures in clinical trials and the process could be made faster and cheaper.

Drug discovery

The feedback driven drug discovery process initiates from the already existing data available from various sources such as high-throughput compound and fragment screening, computational modelling and information available in the database. Initial step in the drug development is the identification of the novel compound with biological activity. The initial compound that exhibits the activity against the biological target is defined as hit which are explored during the screening of chemical libraries, computer modelling or from natural sources. This hit compounds undergoes various screening procedures in cell- based assays simulating the diseased state and in experimental animal models of disease for evaluation of its efficacy and its safety profile. Once hit is studied, the identification of the lead is the next step in drug development. Lead molecule is a chemical compound that has therapeutic properties and can be structurally altered to get a new drug with maximum therapeutic effect and minimum potential of toxicity.

Applications of AI in drug development

Finding successful compounds that can be developed into a new drug is difficult and time-consuming part in the whole of drug development. Incorporating AI in the technologies in various steps of drug development has become versatile and ubiquitous. AI can be applied during finding and validation of drug targets, designing of new drugs, repurposing of drugs, decision making process for selection of patients for clinical trials and improving the R &D efficiency. This can minimize the inefficiencies and uncertainties and also can reduce the bias and human intervention that exist in the classical drug development process.

Apart from this AI can be applied for the prediction of possible synthetic routes for drug like molecules, pharmacological properties, studying the drug combinations, protein characteristics and drug target binding. Also using omics analysis and markers one can identify novel pathways and connections between drug and disease. Deep learning has witnessed benefits in identifying potent drug candidate including predicting their therapeutic properties along with possible harmful effects.

- **AI in understanding the pathway or finding molecular targets**

In drug development, AI has transformed the methods of pathway or target identification to treat diseases. This was possible because of the integration of genomics

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information, biochemical attributes and target tractability. By using AI platforms such as Open Targets and IBM Watson for Drug Discovery one can determine the prediction of drug targets.

- **AI in drug repurposing**

With the use of AI, the drug repurposing has become interesting. Finding existing drugs for treatment of new diseases is always advantageous as the new drug has to directly pass to phase II clinical trials instead of undergoing phase I trial for applying for different indications. In-silico methods predicting pharmacological properties of drug and drug repurposing using transcriptomic data comprising various biological systems and conditions through DL applications were reported.

- **AI in polypharmacology**

Polypharmacology is the concept of one-disease–multiple-targets. This is possible by the greater understanding of the pathology of the disease at molecular level. With the use of various databases such as PubChem, ChEMBL, DrugBank, ZINC and PDB it is possible to collect information of molecular pathways, binding affinity, drug target and biological properties of the drug.

Drawbacks of AI in drug discovery

- AI still cannot replace a human scientist entirely in the drug development process
- The algorithm should clearly lay out the criteria that should be used to parse out meaningful information when the results are in the gray zone of interpretation
- The process is not entirely objective as it can suffer from algorithm bias according to the creaters' own bias in the way the information is processed.
- Establishment of AI technologies requires significant investment.
- Verification of the predictions should be done finally by the scientist to confirm the validation

Conclusion

Interestingly, experts strongly believe that AI will permanently change the pharmaceutical industry and the way drugs are discovered. Currently there is no drug tat is developed by AI application. But based on the advances can be predicted it will take further few years for a drug to be developed using AI. Training of algorithms and domain expertise is still lacking. Although AI can speed up the process real experiments need to be done for validation of the data. Additionally, AI can be used in assisting gene therapy or other therapies that are

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currently not available to us as tools in healthcare. With AI, the possibility of combining regenerative medicine with pharmacology and gene therapy emerges

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