

Artificial Intelligence: Review and Wide Applications in Pharmaceuticals

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Abstract: In life sciences the next frontier is artificial intelligence in pharmaceuticals. Artificial intelligence having a problem-solving ability which comes under the branch of computer and engineering sciences. Basically artificial intelligence is the machine learning program which is much needed now a days in the pharmaceutical industry. In pharmaceutical research and development it should be needed in drug discovery department, to predict the new drug molecule development and also much more needed in evaluation studies of drugs and other biological molecular models. Also the use of artificial intelligence also may improve the process of drug discovery, process of clinical trials and further more studies.

Keywords: need of artificial intelligence (AI), machine learning program, ease of process

1. Introduction

Change matter in every human beings life, like that change is important in various process and various departments, so in field of pharmaceutical sciences and medicine also change is much needed in drug discovery aspects, compounding of chemical products and also manufacturing process of new chemical entities. And artificial intelligence is the one of the innovative process which may change the various aspects of pharmaceuticals for the beneficiary purpose of pharmaceutical sciences. There is need of development of novel and innovative principle and interpretation techniques in mechanical and chemical innovation of pharmaceuticals. The use of automated algorithm program which is the most important part of artificial intelligence (AI) in pharmaceutical sciences to carry out various trials is also very beneficial in case of drug discovery.

History of Artificial Intelligence (AI)

The artificial intelligence program first designed in 1955 by two persons Simon and Newell, and the John McCarthy is the person who also known as father of artificial intelligence, who introduced the term artificial intelligence to the world. There are about four types of artificial intelligence are reactive machines, theory of minds, self-awareness and limited memory.

Artificial Intelligence in Pharmaceutical Research and Development

Artificial intelligence mainly useful in pharmacy for drug discovery, data analysis of new chemical entity, prediction of novel drug products, clinical trials related aspect studies, diagnosis of various disease conditions.

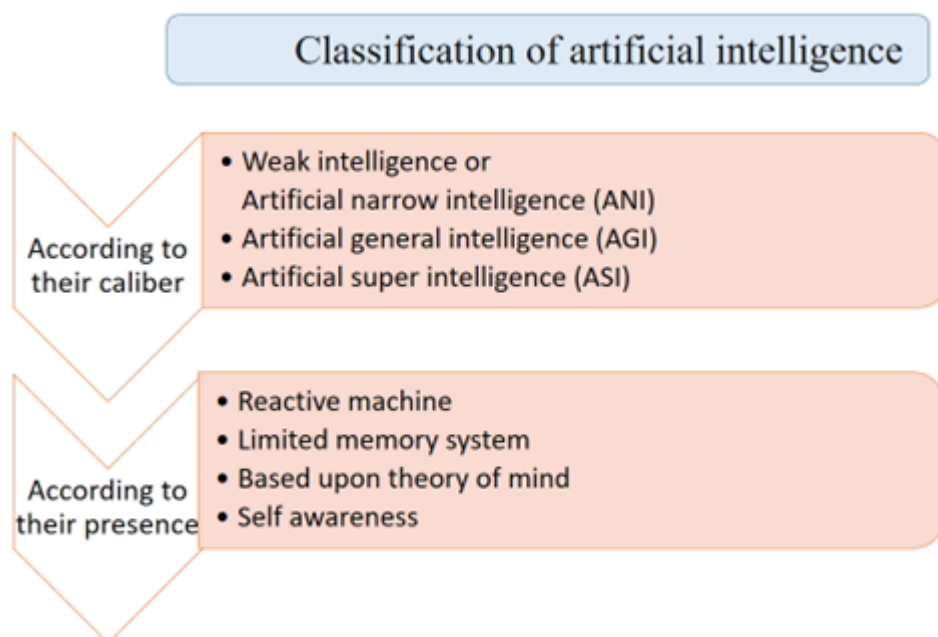


Figure 1

Advantages of artificial intelligence in pharmaceuticals:

- The AI i. e. artificial intelligence gives the results with more accuracy and precision
- Artificial intelligence helps or assist to decrease the errors in the various process which are involved in pharmaceuticals.
- Artificial intelligence technology is more capable to investigate various things by repairing all errors which are caused by human beings.
- the adverse effects and other health risks associated with the medication regarding the condition of patients and analyse with the help of AI program

Disadvantages of AI technology:

- Maintenance and repairing and Complex designing of machine, are highly cost effective.
- The features of Humans have the ability to hear, see, feel and think. They can use their creativity as well as thoughts. These features are not achievable by the uses of machines.
- Human workers may lose their working habits and creativity as because of the undesirable unemployment.

AI - based computer assisted tools used in drug discovery:

- Chemputer: More standardized set - up for reporting chemical synthesis
- ODDT: For use in chemo informatics and molecular modelling
- ORGANIC: Molecular generation tool to create molecules with desired characteristics
- DeepChem: A python - based AI tool for drug discovery predictions
- DeepNeuralNet - QSAR: Predictions of molecular activity
- Neural Graph Fingerprints: - fingerprint Property prediction of novel molecules
- Hit Dexter: Machine learning models for the prediction of molecules, which might respond to biochemical assays

- NNScore: Analysis of neural network - based scoring function for protein–ligand interactions
- DeepTox: Prediction of toxicity and biocompatibility
- PotentialNet: Ligand - binding affinity prediction based on a graph convolutional neural network
- REINVENT: Molecular de novo design using RNN and reinforcement learning
- DeltaVina: A scoring function for rescoring protein–ligand binding affinity
- AlphaFold: Prediction of protein 3D structure prediction

Use of artificial intelligence in pharmaceuticals:**1) Formulation of pharmaceuticals:**

The artificial intelligence technology used in used in the formulation of controlled and immediate release tablets.

2) Development of new products:

The process of pharmaceutical product development is a variate optimization problem. It involves the various process variables and optimization of formulation.

3) In preparations of solid dispersions:

The AI assisted modelling established an appropriate prediction for the preparations of drugs with solid dispersion and with desired dissolution properties with physical stability.

4) For development of Emulsions and micro - emulsions:

Artificial intelligence have also been used for the formulation development of stable emulsions (oil/water) and also for the optimization of the fatty alcohol concentration to formulate emulsions (oil/water) was analysed in this work.

5) For the formulation of tablets, Multiparticulates (beads, microparticles and nanoparticles):

AI is used in formulation and development of multiparticulates (beads, microparticles and nanoparticles)

In Drug Discovery:

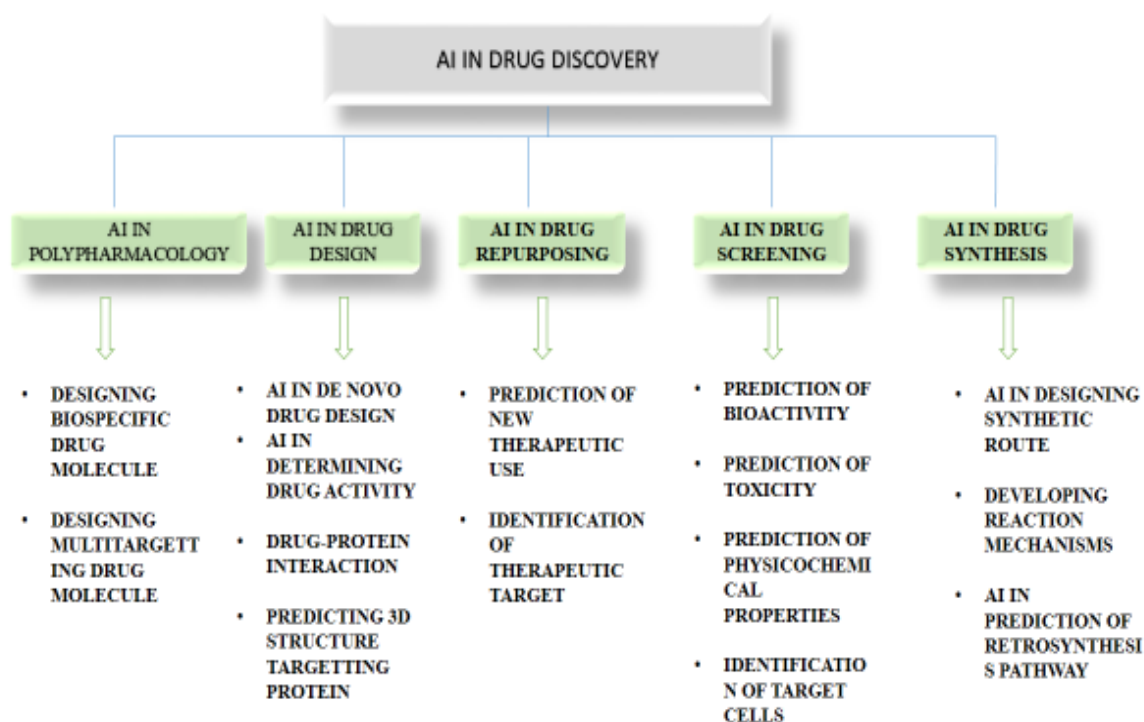


Figure: Applications of AI in Drug Discovery

2. Conclusion

The AI technology is very useful in pharmaceuticals, as the uses of AI technology has been analysing and interpreting some fields of pharmacy like dosage form designing, polypharmacology, drug discovery, hospital pharmacy etc., Artificial Intelligence provide accurate information on patients and expected outcomes with successful result obtained by worldwide data.

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