JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT AT EVERY PHASES

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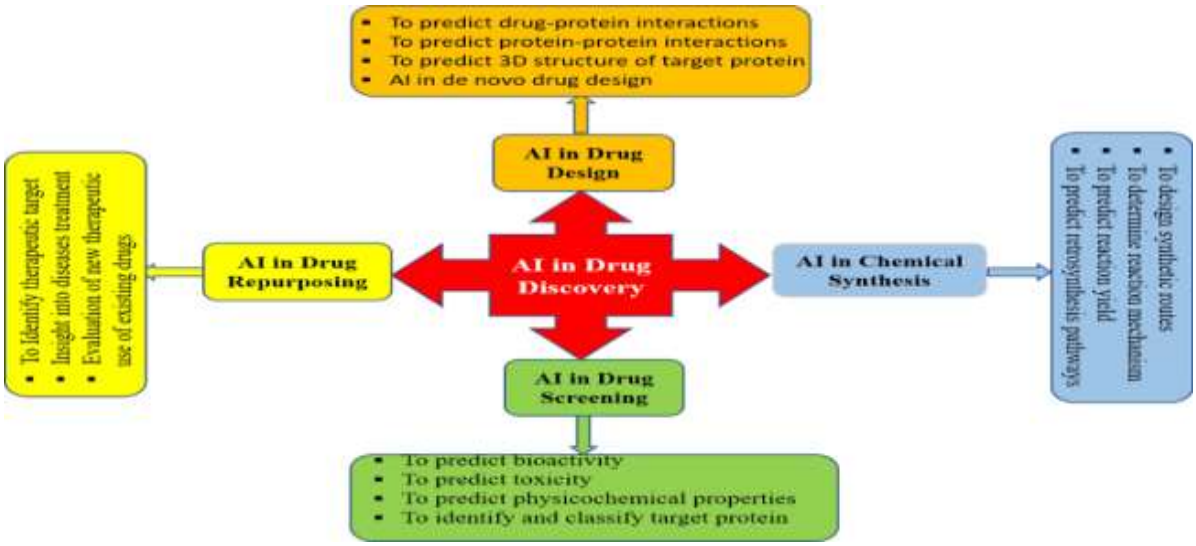
ABSTRACT

The introduction of a new drug to the commercial market follows a complex and long process that typically spans over several years and entails large monetary costs due to high attrition rate. Because of this, there is a need to improve this process using updated technology such as artificial intelligence. Artificial intelligence used in various fields of drug discovery like discovery of new modifications, Preclinical Research, clinical development, FDA review, post marketing. And also, artificial intelligence can help test the adverse effects, side effects or toxicity of candidate drugs. Traditional drug discovery methods or target driven, which means that a known target is used to screen for small molecules that interact with it or affect its function in cells. However, due to complexity of cellular interactions and lack of knowledge of cellular pathways, these are minimal artificial intelligence in drug discovery market can overcome these obstacles. By detecting novel interactions and determining the functional significance of various cellular pathway components. Artificial intelligence has the potential to save more than 70 billion U.S. dollars in drug discovery costs by 2028. According to market research from Berkly. Artificial intelligence can speed up. Drug discovery by finding new insights into a disease, finding possible effects of a drug by testing molecular compounds, repurposing existing drugs, manipulating genetic material.

KEYWORDS: -Artificial Intelligence, Neural networks, Drug Design, Drug Repurposing, De novo Design, Drug screening, Clinical Trails.



INTRODUCTION: -

Artificial intelligence is the ability of a computer or a robot controlled by a computer to do tasks that are usually done by humans because they require human intelligence and wisdom. It's estimated by the. McKinsey global institutional that 75% of companies could be using some form of artificial intelligence by 2025. It is highly profitable for young professionals to learn artificial intelligence to build up their career. Drug discovery is not everyone's cup of tea or coffee. Developing a new drugs course and average of nearly 2.6 billion dollars, and may take as long as 1.5 decades. Artificial intelligence plays pivotal role in circulating these someone timeframe. Artificial intelligence is showing the potential to be faster. More efficient way to find and develop new drugs, a growing number of organizations and universities are focusing to minimize the complexities involved in classical way of drug discovery by using artificial intelligence computing to envisage which drug candidates are most likely to be effective treatment at current scenario.

Artificial intelligence helps in drug discovery and development at various stages, initial from dust, drug discovery, Preclinical Research, clinical studies to post marketing studies. Pfizer is one of the top grossing pharma companies of the world using artificial intelligence to accelerate. Drug discovery during Corona break artificial intelligence helped in discovery and production of COVID vaccines and its role in this is huge. Artificial intelligence can assist in structure-based drug discovery by predicting the 3D protein structure. Because the designs in accordance with the chemical environment of the target protein site. Thus, helping to predict the effect of a compound on target along with the safety consideration before their synthesis or production. Key applications of AI in drug discovery include virtual screening, de novo drug design, retrosynthesis and reaction prediction, they can be reduced to two categories, i.e., predictive and generative tasks. AI works on principal of machine learning models to deep neural networks, such as convolutional neural networks, recurrent neural networks, graph neural networks and transformers.

During preclinical development stage of drug discovery, potential drug targets are tested on animal models using artificial intelligence. During this phase could help trials run more smoothly and allow researchers to predict how a drug will interact with the animal model more quickly and successfully. Artificial intelligence as the potential to streamline the operational process of clinical trials by allowing sponsors and contract research organizations to track patient health from their homes, monitor response to treat and help keep on top of patient engagement. The technology can also predict which patients will benefit from treatment and those that could be at risk and could even circumvent the need for placebo-controlled arms and animal models. Artificial intelligence can help with monitoring during clinical trials by generating your extensive set of data faster. And it can be. Also help with retention by personalizing the trial experience. As a result, artificial intelligence can quickly identify many compounds in a relatively short period under quarter of the cost of traditional methods. The role of artificial intelligence in discovery is expected to grow in the market from 2020 to 2027 due to an increase in the number of cross industry collaborations, increase in venture capital investments, increase in our and activities for the use of artificial intelligence technology, AI-powered drug repositioning, which repurposes existing drugs or drug combinations for new indications they rise importance of drug discovery and

development. Artificial Intelligence is attractive for drug discovery because it applies the rapid and massive number crunching capabilities of 21st century computing technologies such as machine learning to data comparison and analysis in the way the human brain would. But in a fraction of their time. Religions can be used effectively in different parts of drug discovery, including drug design, chemical synthesis and drug screening, Poly pharmacology and drug repurposing. In complex drug discovery. Artificial intelligence has the potential to make processes faster and more cost effective with the hope of reducing the time a new drug needs to reach the patient. Artificial intelligence is used in the pharma industry to manage the process of clinical trial databases. It manages all the clinical trials databases and maintained, organize and store the data in their database.

Artificial neural network: -

Artificial neural network also called as neural networks, are data processing system influenced by biological neural networks that constitute human brains. An artificial neural network is based on a collection of connected units called artificial neurons, which mimic the neurons in biological brain. Each connection is like neural synapse in biological brain is able to transmit a signal to other neurons. An artificial neuron receives a signal then process it and can signal neurons corresponding to it, neurons or aggregated into layers. Different layers perform different tasks on their input signals travels from first layer (the input layer), to the last layer (the output layer), possibly after traveling the multiple layers multiple times. There are three major neural networks, they are convolutional neural networks, Recurrent neural networks and Graph neural networks

a) Convolutional neural networks: -

Convolutional neural networks are mainly used to covert pixels of data in images to reliable data and they share data from different filter which reduce processing time decreasing memory consumption and increasing computation speed. They are used to predict the bioactivity profiles based on microscopy images Convolutional neural networks are also used for molecular property prediction. They also help in learning molecular representations.

b) Recurrent neural networks: -

Main purpose of Recurrent neural networks is processing sequential data. Recurrent neural networks mainly take the SMILES strings as input for molecular property prediction and molecule generation. Multiple connections are present and signal passes over several times for processing, they mainly deal with data extraction from language modeling and music generation. Recurrent neural networks can also be used for molecule generation, parallel to language models for text generation.

c) Graph neural networks: -

It is recently developed neural networks. They deal with the data extraction from graphs and representation of data in graphs. There are two major types of graphical neural networks. They are recurrent Graph neural networks and convolutional Graph neural networks. Main role of graph neural networks is molecular property prediction and for molecule generation.

ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY: -

1)Artificial intelligence in drug design: -

Structural Based drug design includes approaches such as molecular docking, virtual screening, structural based pharmacophore modeling, and de Novo drug design. Whereas lbdd approaches include similarity-based screening, quantitative structure activity, relationship modeling, ligand-based pharmacophore modeling. And scaffold hoping drug discovery applies to a vast range of technologies in interest of assuring new chemical entities of disease relevance into the meat as yet unmet patient needs. While many of technology methods use experiments, is so called wet laboratories, the development and applications of computational methods. Often called in silico as opposed to in vitro in vivo have been in wide usage for many decades. Recently, however, a renaissance of artificial intelligence and specifically machine learning approaches have led the vanguard of novel. Applications to speed drug discovery not only in efficiency gains, but also in development of improved medications for patients. This article contains a number of different and new approaches to applying artificial

intelligence and machine learning methods in drug discovery, sometimes with entirely new algorithms, but often times building on years of research and applied a new added by comment algorithm improvements, but also significant improvements in software. on the hardware that allows. inaccessible quantities of computational power.

a) Artificial intelligence in target protein structure prediction: -

As protein structure data becomes more prevalent due to protein crystallography becoming a routine asset type in drug discovery, new methods arise that incorporate these more sizable data sets to offer more protein binding site contextual information rather than that merely implied by ligand structure data alone. Methods included in structure based predictive modeling or predicting protein ligand molecular organization approaches to using convolutional neural networks in virtual screening and applying machine learning methods in enhancing the impact of molecular dynamics simulation. Artificial intelligence identifies compounds that could bind to undruggable targets, that is proteins whose structure are not defined. In developing drug, it essential to assign accurate target for successful therapeutic activity many proteins involved in formation of disease and they are overexpressed so it is essential to predict target protein structure to design drug molecule artificial intelligence helps in structural based drug discovery by analyzing 3D protein structure along with chemical environment of target protein sight so it will compound on the target with safe considerations. Artificial intelligence will analyze the distance between functional groups and it will also predict the angles to predict 3D target protein structure it will predict correctly 25 out of 43 structures. southwestern and University of Washington researchers led an international team that used artificial intelligence and evolutionary analysis to produce 3D models of Eukaryotic protein interactions. The study, published in science, identified more than 100 probable protein complexes for the first time. And provided structural models for more than 700 previously uncharacterized ones, insights into the ways pairs or groups of proteins fit together to carry out cellular processes could lead to a wealthy of new drugs targets.

b) Artificial intelligence in Drug protein interaction: -

To bring out success in therapy drug protein interactions plays a vital role .to understand the efficacy and effectiveness of the drugs, the prediction of interaction of a drug with the receptor is very essential. Which allows for repurposing of drugs, and prevents Poly pharmacology. Ligand protein interactions and for ensuring better therapeutic efficacy, the various artificial intelligence. Methods have been successful and accurate in production. To avoid Poly pharmacology and repurposing of existing drugs, artificial intelligence as the ability to predict drug target interactions. It is Very crucial to identify novel drug protein interactions for drug discovery. Small proteins produced by the immune system can attach it to specific parts of a virus to neutralize it. As scientists continue to battle SARS-Cov-2 the viruses that causes COVID-19, one possible weapon is a synthetic antibody that binds the viruses spike protein to prevent the virus from entering a human cell. To develop a successful synthetic antibody, researchers must understand exactly how that attachment will happen. Proteins will lumpy 3D structures containing many folds can stick together in millions of combinations, so finding the right protein complex among almost countless candidates is extremely time-consuming. To streamline the process, MIT researchers created a machine learning model that can directly predict the complex that will form when two proteins bind together. Their technique is between 80 And 500 times faster than state of the art software methods and often predicts protein structures that are closer to actual structures that have been observed experimentally. This technique could help scientists better understand some biological processes that involve protein interactions like DNA replication and repair. It could also speed up the process of developing new medicines. Deep learning is very good at capturing interactions between different proteins that are otherwise difficult for chemists or biologists to right experimentally. Some of these interactions are very complicated and people haven't found good ways to express them. This deep learning model can learn these types of interactions from data.

c)Artificial Intelligence in De novo Drug Design: -

AI methods bear potential for early drug discovery and computer-assisted medicinal chemistry. To reduce synthetic efforts and obtain natural product inspired by active small molecules Computer assisted De novo design of natural product mimetics offers a viable strategy but suffers from several limitations. Artificial

intelligence which includes deep learning techniques can help address these shortcomings. Artificial intelligence helps in various methods of De novo drug design like:

* Data preparation and Generative machine learning model

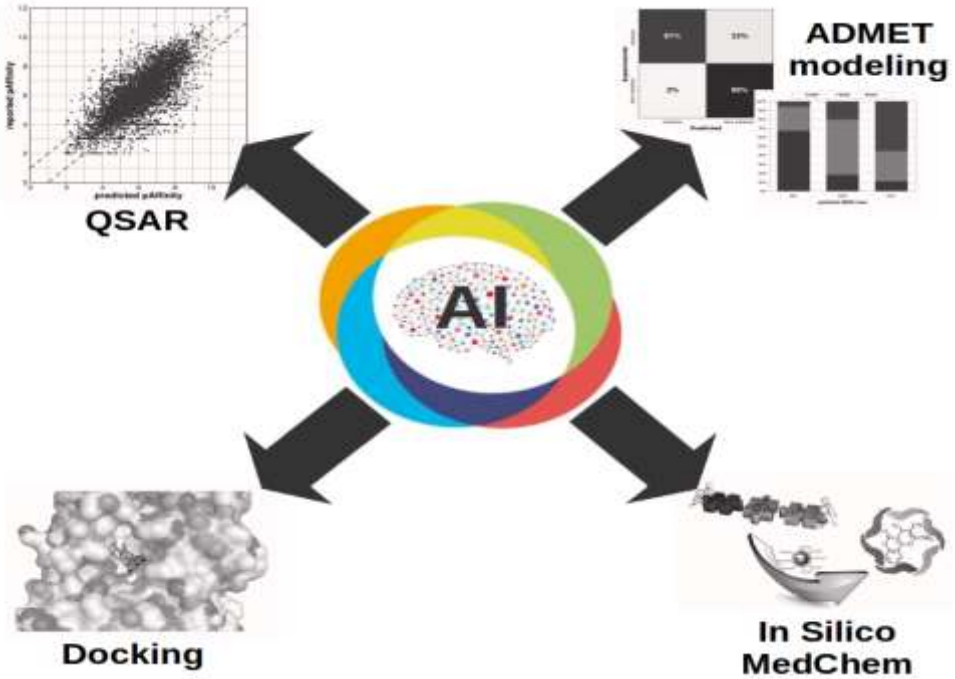
* Similarity searching with holistic molecular descriptors

* Self-organizing map consensus for target prediction

* Scaffold and similarity analysis

* Hybrid reporter gene assays for RXRα/β/γ activation

Artificial intelligence helps in translating the input subsystems into the Latent space permits Which ability to search for similar structures and sampling. From the latent space of generation. Artificial intelligence helps in various experimental section like method overview, learning a latent embedding data. Similarity search. Experiment data generation and modeling training, progressive training, Stacked generators. Interpolation etc.

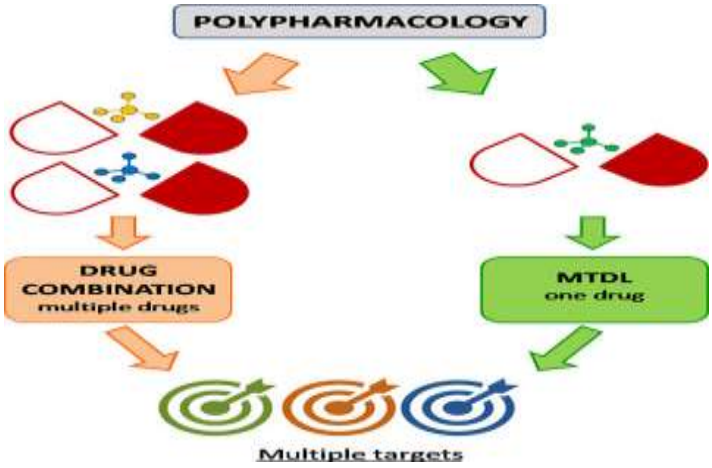


2)Artificial intelligence in Poly pharmacology: -

The concept of Poly pharmacology involves the interaction of drug molecules with multiple targets, which may interfere with the single or multiple disease pathways. The Poly pharmacological studies could uncover new off targets for the existing drugs. Often interact with multiple targets coined as, Poly pharmacology and unintended drug target interactions could cause side effects. Poly pharmacology phenomena include 1) single drug acting on multiple targets of a unique disease, pathway, or 2) single drug acting on a multiple drug targets pertaining to multiple disease pathways. In addition, Poly pharmacology for complex diseases is like lead to employ multiple drugs acting on different drugs. Targets that are part of networks regulating various physiological responses. Only pharmacological approaches aim to discover the unknown of targets for the existing drugs. It is also known as drug repurposing. The approach needs the systematic entry, integration of data derived from different disciplines, including computational modeling, synthetic chemistry in vitro or in vivo. Pharmacological testing and clinical studies. In drug discovery and development, Poly pharmacological studies are critical. High level data. Curation or integration and methodology development from various drug discovery disciplines would be needed for accurate prediction of Poly pharmacology prediction and rational design of multi target agents.

a) Artificial intelligence helps in designing bio specific drug molecules

b) Artificial intelligence help in identifying and designing multitarget drug molecules.



3)Artificial intelligence in drug Repurposing:

Drug repositioning also referred to as drug repurposing or drug reprofiling, is the process of uncovering new Indications of the approved or failed or obtained compounds for use in a different disease. Repurposing will reduce the drug development timeline as various existing compounds have already demonstrated safety in humans. It does not require phase one clinical trials. Potential for reuse despite evidence of adverse effects and failed efficacy in some indications. Aspirin was the first drug to be repurposed. Intelligence algorithms can be used for drug, drug repurposing which is a rapid and cost-effective way to discover new therapy options for emerging diseases. According to Mount Sinai School of Medicine's Covid 19 drug and Gene set library, at least 81 studies have focused on computational drug repurposing for covenanting, compared with 27 studies based on experimental screening data nine months into the pandemic, they remain, say. Paucity of confirmatory data on any of the repurposed drugs, for example the antiviral activity of Remdesivir, one of the most prominently discussed drugs repurposed for SARS, COV-2, has been independently shown in just six independent studies for ten other repurposed. Drugs. Only one further confirmatory study has been published since the initial report.

This illustrates the uncertainties regarding reproducibility and rigorous evidence with respect to source code to and drug repurposing facing the scientific community and other applications of artificial intelligence. Or machine learning aims to identify patterns of viral spread and disease course likelihood in different patient groups. According to Milken Institute, at least 20 efforts to repurpose drug candidates are underway, some using experimental approaches and others using artificial intelligence or machine learning, or a combination.

a) Artificial intelligence helps in identification of therapeutic targets in drugs.

b) Artificial intelligence helps in prediction of new therapeutic use of drugs.

4) Artificial Intelligence in Chemical Synthesis: -

In organic chemistry, artificial intelligence is driving one of the most important revolutions. Multiple platforms Including. Synthesis for reaction prediction on machine learning, have successfully become part of the organic Chemistry Daily Laboratory assisting in specific synthetic problems. Artificial intelligence helps in reaction prediction and retrosynthetic models. The prediction of reaction yields as received less attention in spite of the huge potential of accurately predicting reaction conversion rates. Artificial intelligence predicting reaction yields could support synthetic chemists in choosing an accurate synthesis route among many predicted by data driven algorithms and also Reaction yields prediction models could also be used as scoring functions in computer assisted retrosynthesis route. Planning tools to complement forward prediction models and in scope filters. Organic chemistry Chemical reaction involves Reactants and products which are separated by an arrow in written structural form by using some of the catalysts under particular temperature and ph. Artificial intelligence make these complex reactions into simpler form along with side reactions. AI helps in chemical transformations capable of converting all reactant molecules into products with maximum yield possible. Present in organic chemistry. Some chemical reactions are by lower or higher yields with the actual value depending on reaction conditions like temperature, concentration etc. And on specific substrates. It is game changing asset for estimating the reaction yield. It gives chemists with the maximum ability to evaluate the yield

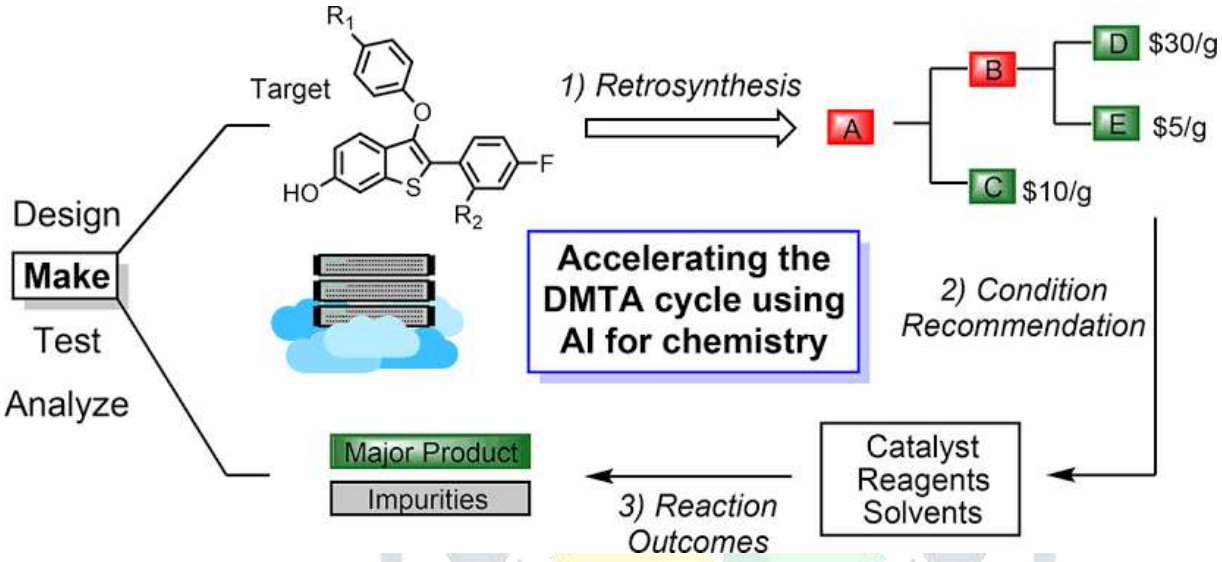
of complex reaction paths. With the possible shortcomings of investing hours and materials in wet lab experiments. Artificial intelligence is also being used in material science and physical chemistry, where the two disciplines are aiming to predict functional materials, structural property relationships, and chemical process optimization. Program synthesis is the idea of automatically generating programs from specifications. It is different than program verification. Eventually, researchers of artificial intelligence in the 1960s elaborated on the concept of program synthesis to applying it to symbolic artificial intelligence. Research. Artificial intelligence has accelerated the synthesis and production of COVID-19 Vaccine recently. Artificial Intelligence helps in retrosynthesis. Prediction of chemical synthesis by deep learning is one of the major Importance.

a) prediction of reaction yield.

b) Prediction of retrosynthesis pathways.

c) developing Insights into Reaction mechanisms.

d)designing synthetic routs



5) Artificial intelligence in Drug Screening: -

The process of finding a new drug against a chosen target for a particular disease. Usually involves high throughput screening (HTS). Wherein large libraries of chemicals or tested for their ability to modify the target. The drug screening is the process by which potential drugs are identified and optimized before selection of a candidate drug to progress to clinical trials. It can involve screening large libraries of chemicals for a particular biological activity in high throughput screening assays drug screening is a more cost-effective approach as it is relatively cheaper than a drug test.

Artificial intelligence also helps in predicting the prediction of bioactivity and also identification and classification of targeted cells.

a) predicting toxicity: -

Pharmacology of the drugs are one of the most Potent weapons against the diseases. drugs usually have some of side effects and adverse effects along with therapeutic activity. Pharmacovigilance the pharmaceutical field which will monitors, detects and prevents the side effects and adverse drug reactions. Safety effects begin during development process using in vitro and in vivo studies whereas in vitro is preferred over in vivo. Analysis Continue through clinical trials and it will lead to post marketing surveillance of adverse drug reactions in populations, future toxicity and safety challenges include increased polypharmacy and patient related problems. Massive amounts of newly available data present an opportunity for using artificial intelligence and machine

learning to improve drug safety science. Here we explored recent advances as applied to preclinical drug safety and post marketing surveillance, with a specific focus on machine and deep learning approaches.

b) prediction of physiochemical property: -

Physicochemical properties which include solubility, degree of ionization, partition coefficient, intrinsic permeability of drugs. These will affect the pharmacokinetic properties on target receptor family, hence must be considered when designing a new drug. To predict physical chemical properties, different artificial intelligence-based tools or used for example. Machine learning uses large data sets produced during compound optimization done previously to train the program. Physiochemical properties of molecules which are based on theories and analytical proof vast data are taken into consideration and combination properties such as interaction bioavailability can be predicted. Artificial intelligence helps in predicting stability pH and drug absorption. The stability pH profile is a plot of the reaction rate constant for drug degradation versus ph. If drug decomposition occurs by acid or base catalysis, some prediction of degradation of the drug in the gastrointestinal tract may be made. For example, has a pH dependent stability profile in acidic medium as in the stomach Christmas in decomposition occurs rapidly, whereas in neutral or alkaline pH the drug is relatively stable.

Artificial Intelligence not only helps in drug discovery but as vast uses including preclinical trails, clinical rails and pharmaceutical manufacturing and quality analysis, pharmaceutical product development and management. The lipophilicity and solubility of various compounds are predicted by using ADMET and ALGOPS program of neural networks. To predict the acid dissociation constant of compounds predicted by kernel ridge-based models and graph kernels and ANN based models. To generate cellular permeability data of diverse class of molecules by AI assisted predictors.

6) Public Data Resources: -

They are source of publicly available data resources. They mainly provide information related on molecular structures, molecular properties and target information such sites are as follows, PubChem,ChEMBL, ZINC are leading platforms and author such platforms are PDBbind, BindingDB, DUD, DUD-E, MUV, STITCH, GLL&GDD, NRLiST BDB, KEGG. PubChem was launched by National Institutes of Health in 2004.As of August 2020, PubChem contains 77 million SMILES,111 million unique chemical structures with 271 million activity data points from 1.2 million biological assays experiments. ChEMBL is under European Molecular Biology Laboratory, is another large-scale chemical database which contain 1.6 million distinct chemical structures with over 14 million activity values it also has web application program interface.

7) Benchmark Platforms: -

They are used for evaluation of molecular property prediction and molecule generation. The benchmark datasets cover four categories: a) Quantum mechanics b) Physical chemistry c) Biophysics d) Physiology involving single task or multi tasks. REINVENT developed by Olivecrona in 2017, which is a sequence-based generative model utilizing SMILES strings. REINVENT strives for generating analogues and generating ligands for a given target. A more recent evaluation platform MOSES was released by Polykovskiy in 2020, which contain a list of metrics for detecting common issues in generative models. MolMapNet was released recently. MolMapNet also explains the Molecule Net by adding pharmacokinetics-related information.

Artificial intelligence in clinical trials design and monitoring: -

AI plays an important role in clinical trials by generating a more extensive set of data faster and it can also help with retention by personalizing the trail experience and risk. It will predict and analyze the subject enrollment and selection of volunteers in clinical trials this technology can also predict which patients will benefit from treatment and that could be at risk. It also allows the sponsors and contract research organization to track the patient health. It helps in monitoring the trail and patient dropout.

AI in pharmaceutical manufacturing and development: -

AI helps in automated manufacturing of the drugs in industries and also used in personalized manufacturing and it will give the indication of errors in manufacturing unit by corelating manufacturing errors and it will set the parameters to correct it. It will hasten the production process with minimum errors and more efficacy. Artificial

intelligence in product. Development will help by deciding suitable excipients and monitoring and modifying development process and ensuring in process specification compliance.

Artificial Intelligence in post manufacturing process: -

The post manufacturing processes, which includes. Quality assurance, quality control and pharmaceutical product development and pharmaceutical product management and post marketing also plays important role in drug processes. artificial intelligence in. Quality assurance and quality control. Will help by understanding critical processes parameters and it will guide future production cycle and by regulation of in line quality and it will also ensure quality assurance with aid of ECN and other techniques. Artificial intelligence in pharmaceutical product management. Will predict the market positioning. And market prediction and analysis. And it will also analyze the product costing.

In future, artificial intelligence plays a vital role in drug discovery and development. 75% of the world pharmaceutical companies will use artificial intelligence in drug discovery and production by 2028.

Conclusion: -

From this review article, we come to know about the importance of artificial intelligence in drug discovery and development and its wide applications in various fields of drug manufacturing and production. In the field of drug discovery Artificial intelligence has received much attention compared to traditional method of drug discovery. A based drug discovery methods are more beneficial because these are data driven, complex algorithm and machine learning can extract meaningful information from a large data set and it can also identify compounds that could bind to undruggable targets i.e., proteins whose structure are not defined.

Artificial intelligence has higher predicted Power to defend meaningful interactions in their drug screening, therefore the potential for errors, which can be reduced by careful designing the parameters of assay questions. Most importantly artificial intelligence has the potential to move drug screening from primary stage to virtual lab. Where results of a screening can be obtained with higher speed and Accurate targets can be listed without need for exclusive experimental data and manpower. Artificial intelligence uses the high advances in biology and computing to develop state of the art algorithms for drug discovery. With the increase in processing and reduction in processing costs. Artificial intelligence has the potential to level the playing field in drug development. Though, artificial intelligence plays an important role in the drug discovery, but it cannot entirely replace the human scientists in the process of drug discovery.

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