

Using Artificial Intelligence for The Design of Polymeric Drug Delivery Systems

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Abstracts

AI is cost effective and time efficient process. Artificial intelligence is a method which uses high speed calculation, the improvement regarding algorithm along with collection about biological and chemical features in pharmaceutical exploration and development. Present day because continuous progress towards machine learning (ML), Artificial intelligence an effective statistics analysing technology might have been broadly utilized in drug design. In pharmaceutical exploration and research employ of AI in target identification, compound screening, hit to lead identification, preclinical and clinical trials and 3D printing. This review from 2019 to 2023 gives the achievable information on pharmaceutical exploration along the Machine learning devices and methods which implement in each and every stage of drug advancement. The integration of AI and spectroscopy in pharmaceutical exploration has enabled higher target accuracy, reduced toxicity, and improved dosage formulations. This review article elucidates the utilization of AI and chemical engineering at each stage of pharmaceutical exploration. We conclude this article by using extensive literature search, news articles to know the latest position of artificial intelligence in drug advancement. Machine learning, a subset of artificial learning that permit numerous layers depiction of data with several layers of extraction have submit improvement in academic, industry like speech identification, image categorization, bioinformatics etc.

Keywords: Speed calculation, artificial intelligence, chemical tubes, drug design, spectroscopy, polymeric drug delivery systems

INTRODUCTION

John mc carthy in 1956 coined the term “artificial intelligence.” [1]. Artificial intelligence is focusing on set up machines to learn general rule from data, also known as machine learning. Pharmaceutical exploration is a costly and time-intensive endeavour. Furthermore, the success rate of bringing a drug to market, with an approval rate of less than 10%, is notably low [2]. Artificial intelligence is a tool which radical transform pharmaceutical exploration process with increased success rate of approval in pharmaceutical exploration.

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Drug development can be based on following steps:

- i. Choosing and confirmation of target
- ii. Different stage like primary and secondary evaluation and refinement of lead compound
- iii. Pre-clinical studies
- iv. Clinical trials [3].

Pharmaceutical exploration happens when there are no existing drugs available for a particular disease, or when the discovered drugs have limited effectiveness. The very first step in pharmaceutical exploration is target selection and target identification. Target may be gene, protein. Normally target identification and validation takes typically 2-6 months but determining the structure of the target receptor by artificial intelligence that

process occurs faster [4]. AI helps in identifying lead molecules, faster pharmaceutical exploration, and faster drug optimization in pharmaceutical exploration and development. AI essentially sifts through vast amounts of data to forecast potential targets and appropriate candidates for specific diseases [3].

Typically, AI uses algorithms to solve complex problems. AI risk algorithms are used for agent screening and toxicity prediction. AI has the capability to analyze extensive datasets, including pharmacokinetics, resolution profiles, and gene mapping of targets of interest. Insilico medicine® is using the idea of platform like generative adversarial Network and generative tensorial reinforcement learning for identifying potential target [5].

Machine-learning (ML) and deep-learning (DL) are subsets of artificial intelligence (AI). Machine learning and 3D printing understand huge medical engineering data and convert within useful information. Conventional algorithm in ML is Multiple linear regression, Naive Bayesian classifier, logistic regression, Support vector machine and many more used in pharmaceutical exploration process[6] DL is promising and efficient data processing methods.[7] DL mainly uses artificial neural network with composed of non-linear processing units for learning data presentations DL is broad area in AI. Deep learning is the latest and well organised processing method. It rely on deep hierarchial model of data learning. Conventional Machine learning require physical design and removing of featur from raw data. At the same time deep learning use several under wraps layer and neurons those can bring out highest abstract from raw information by using complex algorithm.[7] The utilization of AI technology is creating new opportunities across the spectrum from target elucidation to drug advancement mentioned in Figure 1.

AI operate target pharmaceutical exploration platform and can extract target- relevant information from a large volume of complex ,give a better disease target assosiation,target relvent information ,hence strong link of any disease to target site .[8]

AI : SYSTEMS AND DRIVES

AI requires many approach domain,such as reasoning,comprehension study,explication explore,also amid a basic model of machine learning (ML).ML utilize algorithms which identify design with in a set of data. Enter Artificial Neural Networks, part of deep learning AI. This advanced computational feature requires simulating electrical transmission with the same sensitivity as a human biological neuron (the basic unit of an artificial nervous system) impulses in the brain. Artificial Neural Networks comprise nodes that receive inputs and transform them into outputs. Artificial neural networks come in various types, including multi-layer neural networks, recurrent neural networks, and convolutional neural networks [9].

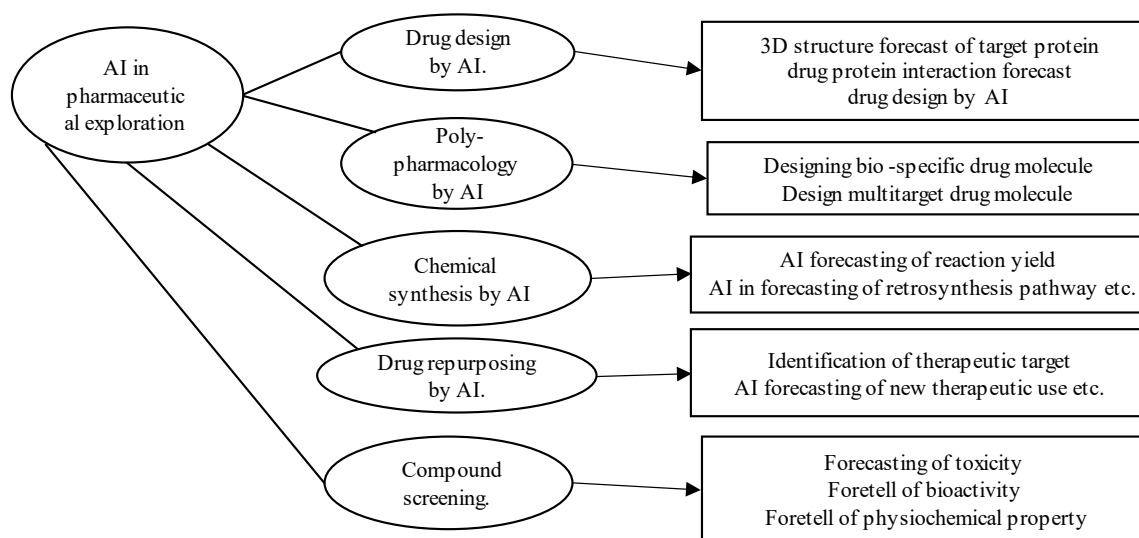


Figure 1. Aspects of artificial intelligence applications[7].

AI In Target Identification And Validation

Essentially, pharmaceutical exploration approaches fall into two groupings: system-based phenotypic screening and target-based design. These categories together have accounted for more than 90% of FDA-approved drug discoveries between 1999 and 2008. Phenotypic screening change phenotype in disease related assay without knowing the target and mechanism of action. phenotypic screening monitor the living cell response which is clinically relevant. A target based approach has been made superior to phenotypic approach. Due to advancement in structural genomic, proteomics, bioinformatics and high through put crystallography many structure has been identified. [10] AI and spectroscopical analysis area has moved from theoretical word to real word. Target selection process in pharmaceutical exploration is very pivotal decision point. Hence, there is a need to improve the target selection process by integrating AI techniques. [11]. Traditionally QSAR is based on statistical method of deep learning but now a days development of novel algorithms is drastically increased. Deepchem is used for several pharmaceutical exploration task Deepchem is written in python language [12]. Innovative techniques such as deep neural network, convolutional neural networks, and recurrent neural networks have been extensively employed in deep learning. [13] To date target identification or target prioritization remains an uncertain process. Although the majority of drug act via a protein targets. The target normally a macromolecules that bascially interact with the therapeutics agent. It is important to map the interactions between the approved drug and suitable target. Targets are those macromolecule through which any therapeutics agent exert their effect. knowledge graph which is a topological method is used to represent the protein function associations. Metapath methodology is used for the novel drug target. Drug target may be human protein ,sugars, nucleic acid,metals lipids shown in Figure 2 [14].

Proteins are fundamental molecules in our body and play a vital role in mediating every function of drugs within the body. While determining the three-dimensional structure of proteins, especially large molecules, through experimental methods can be challenging, small molecules can be easily determined through ligand binding programs such as AlphaFold. AlphaFold is capable of predicting the 3D structure of proteins based on their amino acid sequences. Meta Platforms Inc., the parent company of Facebook, has developed a tool using artificial intelligence to guess the structure of thousands of proteins. This advancement has capacity to enhance scientists' understanding of biology and facilitate breakthroughs in pharmaceutical exploration. Meta AI introduces the latest embedded AI computer program, named ESM Fold, which generates a publicly available database containing predictions for 167 million proteins. Protein is a vital component of life, important for the foundation of tissues, organs, and cells. According to Meta ESM Fold, it is 60 times faster than Alpha-Fold, but more accurate. The ESM Fold index is great because it made forecast from genetic sequence those had not been calculated formerly. Meta research generated the predictions using a form of AI known as a large language model that can predict text from just a few letters or words it is same technology that allows Open AI's Chat gpt to generate humanlike responses [15]. Drug should be bind to multiple protein rather than a single protein for therapeutic effect. Through active learning we can find out the novel compound which have a promising activity against a disease target [16].

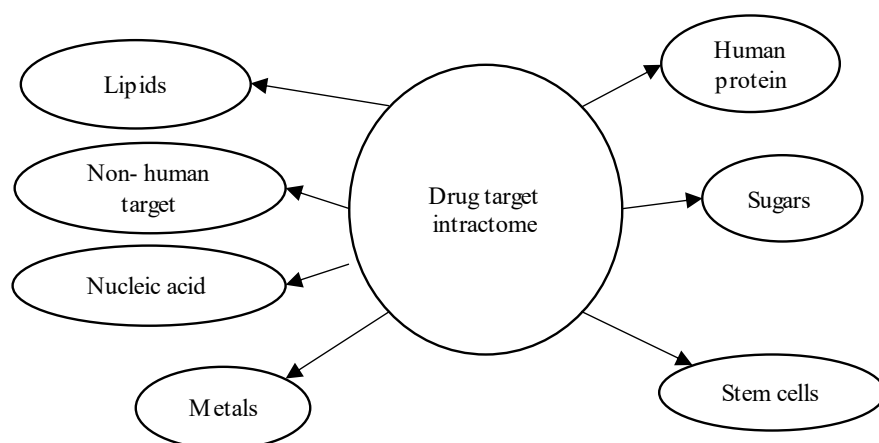


Figure 2. Drugs target categories for different things [14].

In target discovery, a critical step is target's druggability (a target's capacity for therapeutic modulation by medications). Target should have biochemical attributes that permit the molecule which have drug like properties druggability on the basis of machine learning can be found out by Surface Cavity Recognition and Evaluation webserver which detect compound binding and non-compound binding space on protein. Example of AI derived novel targets are protein tyrosine phosphatase, SHP2, DNA Helicase WRN paracaspase (are animal-present proteins connected to caspases), MALT. RNN has been used set up for natural language extracting. But now a days it is used for successful de novo drug design. RNN used as sequential information for input. RNN produce SMILE strings for work together for generation of chemical structure in sequence of letters and generation of chemical structure. Drugs that do not exhibit a bit of cooperation regarding targeted protein inefficient to bring any therapeutic effect. Hence, drug-target binding analysis (DTBA) proves valuable in predicting drug-target effects. Methods like Kronecker regularized least squares (KronRLS), which incorporate both machine learning (ML) and deep learning (DL), are employed to ascertain DTBA. Commonly utilized approaches for this purpose include SimBoost, DeepDTA, and PADME. Similarly, Sim Boost uses regression trees to predict DTBA. DeepDTA takes protein input data from amino acid sequences and SMILES complex statistics to represent 1D drug structures [17].

Primary Screen

Signatures used in low-target recognition, high-throughput virtual screening (HTVS) and bioassay techniques. Understanding the effective site for the receptor to which the ligand binds is necessary to copy the anatomical role required for the function required by initiating HTVS binding. Similarly, the binding-based virtual assay (LBVS) recognizes that an alternative primary approach depends on the biophysical effect of a chemical indicator. The scoring function is a basic element of biological networks to evaluate the similarity between targets. Attributes of mapping capabilities in ML can provide great skills to collect physical, geometric and chemical data to solve problems. The score is created through a data-driven black box design, which predicts interactions and binding forces and revolves around some assumptions in the dock, such as physical functions that are difficult to study. Random forest and SVM concepts are employed within artificial intelligence to enhance the signature function. For instance, an SVM design can replace a linear additive design in relation to the energy phase concept.

SVM can designate the association between experimental obligate affinities and possess energy phase it could be elicited from docking plan. Consequentially, data allow greater performance in scoring ability and screening ability. In the assessment of protein-ligand compatibility, Jimenez et al. perform the "3D visual representation of convolutions neural network design and binding compatibility which have shown greater correlation behaviours in index". DL constitutes his original potency for improves conceptual features from simple features, therefore it is compulsory to constitute basic aspects for a compound like protein make-up like molecule types, particle differentiation etc. Therefore, the mark in activity scoring was, selecting some aspects amid protein-ligand interaction for forecasting binding in pharmaceutical exploration.[18].

AI In Hit Identification

The HIT is the compound that show sufficient activity against any target. HIT is obtained from screening of chemical collection, computer duplication and screening of naturally material like plants and fungi [16]. The biological activity appear when interaction between compound and enzyme occur. Through the procedure of lead initiation, the hit molecules are consistently altered to increase the action and accuracy toward a certain target. Those compounds which are related to hit are stated analogous and this process is known as hit expansion. To enhance the throughput, chemist and researcher focus on a series of reaction for building block. Building block are those compounds that contains a functional group and can easily attach with energetic site of biological target [19]. Energetic site are those which bind to any compound. Energetic site also known as the active site. The attachment of any compound to energetic site is same as induced fit model or lock and key model[20]. Neural Graph Fingerprint is used for discovery of novel compound. Optimization of hit has been done by virtual screening. "AI has

also been utilized in various aspects of virtual screening. Virtual screening is primarily categorized into two types: structure-based virtual screening (SBVS) and ligand-based virtual screening (LBVS)". Molecular docking is a commonly used technique in structure-based functional studies. In the initial docking step, molecules from a library are positioned within the active site of the target based on their steric and physicochemical properties. The scoring function is a mathematical model in which the relational pose is generated by the proximity of the target to the tree. Recently, knowledge-based data mining is an important topic [21]. Estimation is a processing step and is carried out by various software such as matching algorithm, incremental construction algorithm, monte carlo algorithm. The scoring function is not very reliable in the dock approach. A more advanced AI algorithm for structure-based, efficient filtering is the non-parametric signature function. Random signatures like SVI-based ID score, RF-based RF score, and ANN-based NN score play a crucial role in establishing robust connections with enhanced accuracy [22].

AI In Lead Generation and Lead Optimization

The lead identification phase is the subsequent step in drug development. The lead is the compound which have good prospective to treat any disease. After identifying hit they pass through cell-based assays foretelling of disease condition and in animal model of disorder to determine the safety and efficacy of compound. One time a lead compound has been selected its composition is utilize as with the purpose for maximum therapeutics benefits and minimum harmful effect. Lead optimization is very expensive and time taking process [18].

Lead optimization

This phase requires a lot of time to find a cure. Lead optimization is a multi-parameter optimization through which the power combination is sufficiently determined. Safety, efficacy and pharmacokinetic properties are simultaneously optimized from lead compounds. Lead optimization entails the iterative execution of the DMTA (design-make-test-analyze) cycle. Optimizing the efficiency of this cycle and hit detection is facilitated by AI-driven computer-aided synthesis planning (CASP). Chemists can use CASP to determine the most efficient and cost-effective route for synthesizing the target molecule, thus speeding up the "make" phase of the DMTA cycle. The DMTA cycle concludes during the "test" phase.

AI In Synthesis of Drug-Like Molecule

Which compounds follow Lipinski's rule of five called drug -like molecule or compounds.

- Molecular weight of drugs ≤ 500
- Lipophilicity of drug, $\log P \leq 5s$
- Unit of H- bond acceptors ≤ 10
- Unit of H- bond donors ≤ 5

Retrosynthesis approach is used for synthesis of drug-like molecules. The very first step in retrosynthesis intend identify the selective compounds and transform into them small scale building block. Subsequent analyse the reaction that change these smaller building block into target molecules. Following step is quite complicated due to difficulty for human brain to investigate the enormous tally of significant organic reactions obtainable in the literature to collect the most feasible reaction [21]. AI would do away these reactions that develop high failure in organic reactions. At present several computers aided organic compound synthesis (CAOCS) system help to chemist to selecting the best synthesis route. AI platform known as 3N- Monte Carlo tree search (MCT) developed by segar et.al.

AI In Preclinical Studies

Predicting physicochemical properties such as solubility, partition coefficient, and degree of ionization influences the pharmacokinetic characteristics of a drug. Various AI-based tools are available to accurately predict the physicochemical properties of drugs. Algorithms for drug composition rely on molecular descriptors, such as Simplified Molecular Input Line System (SMILES) strings, potential energy measurements, and electron density surrounding the molecule. *In vivo* activity and toxicity detect by algorithm like Nearest-Neighbour classifier, RF, learning machine and deep neural network

(DNN). Neural networks (DNN) are construct as ADMET studies and lipophilicity and solubility profile detect by ALGOPS program.[14] Now a days prediction of ADME/T studies by AI is successfully enhanced. Model planning has been intentionally replaced by AI-based algorithm Linear Multivariate Method (NM) through the original multivariate linear model, including multiple linear regression (MLR) and partial least squares (PLS). Gaussian (non-parametric approach to supervised learning), support vector machine (SVM), Naïf Bayes classifier (NB) and random forest (RF) algorithm is used as a prediction model ADME / T. This model is used to study ADME / T in vitro. In 2013, Lusci et al used an undirected graphical neural network (UG-RNN) to predict molecular structures and applied this method to guess aqueous solutions of compounds embedded in DL networks. [7]. Deeptox is a multi-DNA model for toxicity prediction by Mayr et al. Proctor is used to predict toxicology in clinical trials. The ADME/T study used independent cross-sectional testing and more timely validation by multiple DNAs for small-scale data points. Epoxides metabolite is the main cause of toxicity. By detect the site of epoxidation (SOE) can easily decrease the chance of by-product formation .702 epoxidation reaction database and deep convolutional neural networks (DCNNs) model used by Hughes et al. for accurately foretell regarding site of epoxidation (SOE).[22]

Pharmacokinetics includes absorption, distribution, metabolism, and elimination. Various bioavailability parameters are used to determine the extent of absorption. Various health services describe the improvement of absorption characteristics of bio-availability molecules in the performance of multiple linear regression (MLR) models, Tian et al. Worked on 1014 molecules for bioavailability by molecular credit and systemic fingerprinting. With the use of genetic phenomena such as heredity and the structure and function of DNA, remarkable results appear in predictive work. Steady state drug distribution (VDss) is an important parameter to evaluate drug distribution. Therefore, VDs must, Lombardo and Jing proposed partial least squares (PLS) and random forest method with 1096 molecules. Many AI programs take the details of large drug metabolism to metabolize UDP-glucuronosyltransferases (UGT), cytochrome P450, and others, and train the nervous system in UGT metabolism. Partial rent can be easily estimated using the regression least squares (PLS) method [23].

Ai Application in Drug Repurposing

Drug development and clinical trial within human and animal occur time taken and costly task. Normally, the entire procedure being establishing a latest FDA approved drug needs 10-18 period of long time and huge value of \$2.7 billion. Although, overpriced cost for new drug has not been capable towards enhance the value of drug acceptance. By justifying this limited rate of acceptance, the fundamental aspects of the one-gene, one-drug, one-disease model of conventional drug development continue.

In pharmaceutical exploration there is approach to use of new drug from old one. Drug repurposing is also known as drug repositioning. This strategy is also useful to promising drug candidates that have gone through phase I of clinical trial. AI fast recognise new sign for numerous investigated drugs. AI Bring out novel biomarker and therapeutics targets for existing drugs. AI match existing drug with orphan diseases. AI performs experimental biology by testing over 1000 compounds in 100+ cell disease models [24]. Earlier approved drugs reduce drug development costs and reduce drug safety concerns. Extensive genetic, chemical, and pharmacological data have provided the latest opportunities for drug repurposing. Drug Targeting (DTI) is important for pharmaceutical exploration and therefore medicine. It is important to expect DTIs with computational methods [25].

Ai In Clinical Trial Design and Prediction

The unsuccess rate of clinical trial provide inability of the drug process cycle. Clinical trial can take up to 7-10 years with USD 1.4 -2.0 billion. Great failure occurs due to unfit patient nomination, enrol and incorporate with the ineffectiveness to monitor the patients throughout the trial. IBM Watson has evolved a system for clinical trial matching for utilization of structured and unstructured patient medical data and compare this data with trial eligibility criteria. Failed clinical trials may transpire when there's inadequate and consistent monitoring of patients and clinical endpoints. AI can aid in mitigating these deficiencies in ongoing clinical trial design. AI can discover design the meaning in big data file like

text, speech and images. Human machine interferences (HMIs) and Natural language processing (NLP) permit natural interchange of details between humans and computers. This information may be used for associating big as well as A trial database to better compare electronic health records (EHR), medical literature, and patient trials, and additional trials to monitor patients in trials [14].

Patient Selection

An acceptable patient might not be stage of any ailment, thus creating the patient unsuitable. A 32% failure in phase III is the failure of state of progressive of arrangement in clinical setting. The FDA recognises that the following criteria should be used when choosing a patient group. i) Decreasing population diversity. ii) Selecting patient who are expected to have a quantifiable endpoint. iii) Patient who have predictive enrichment means who are efficient of restoring to a treatment [26,27]. Population diversity may be overcome by electronic phenotyping within health informatic. By using electronic phenotyping patient with special character of interest are selected. Although electronic phenotyping may be important in reducing the heterogeneity of the patient population, it has not been established to improve prognosis. By using ML method for predictive enrichment for neurological disorder which provide simple and cheap biomarker. Patient monitoring is very complicated task in clinical trial. It is important that patient under the examination in clinical trial procedure and regulation during the proceeding of trial and data point for observe the effect of the examine drug and gather well organised.[28] During the trial there is chances of dropout, it requires additional recruitment which effect on time and cost. Patient monitoring can be improved by proper coaching during clinical trial, build endpoint observation more efficient, hence decrease dropout rates. AI techniques with wearable technology provide some access power methodological, mobile, real time, customized patient monitoring system. Through AI, data is captured by wearable sensors and checked in real-time at control points by mobile processors running AI models. Monitoring results are collected locally, in the cloud, or a combination shown in Figure 3.[3].

AI APPLICATION IN DOSAGE AND DRUG DELIVERY

Taking one inadequate quantity of drug to a patient show undesirable and fatal side effect. Therefore, just as important to know a safe and secure drug dose for treatment basis. During past periods it has been complicated to discover the optimum quantity of drug with desired efficacy and less toxic side effect. By arrival towards AI, many of scholars are gaining the assist of Machine learning (ML) and Deep learning (DL) algorithm about suitable drug dosage. Such as AI based platform AI-parabolic response curve (PRC), to selecting the suitable dose for HIV medication by antiretroviral therapy. AI-Parabolic response curve is a neural network operate application, that connected drug combination and dosage quantity to effectiveness across a parabolic response curve (PRS). Through AI parabolic response curve optimum drug dosing can be set up [29].

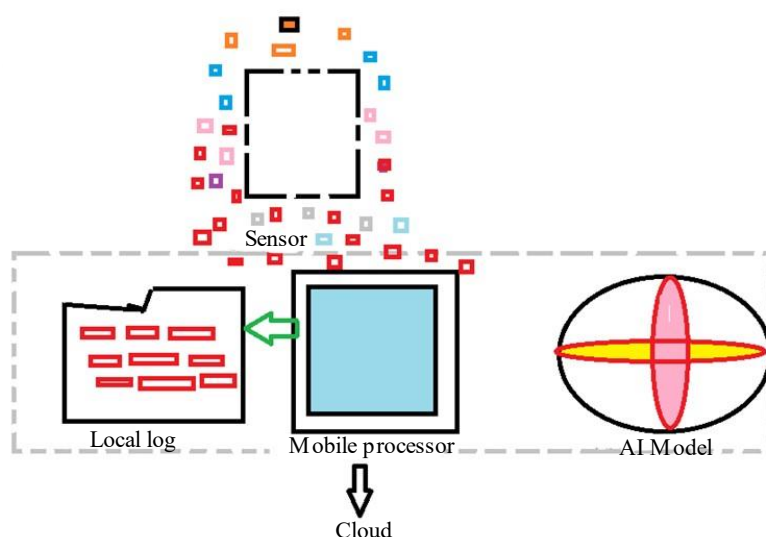


Figure 3. Cognitive sensor to capture real time data[3].

AI Application In Forecast of Bioactivity and Observation of Drug Release

Drug control is a complex and complicated process. Numerous online tools have emerged for assessing the release of new drugs and evaluating the responsiveness of bioactive compounds chosen as carriers. A standard data set was used to validate the statistical analysis. The similarity score based on the chemical attribute is the most similar pharmacophore. This model was successfully tested in silico on a large-scale 3D database. Knowing the bioactive ligand is an important step selecting an effective medication for a particular use. Now, scholars use the benefits of AI in making decisions on bioactive compounds because they can be used for specific purposes related to diseases [30]. Similarly, Wu et al. . Chiçonska et al. utilized a two-dimensional double nuclear method to assess the bioactivity of the compounds. Additionally, Merget et al. highlighted the importance of identifying adverse drug reactions (ADRs) in the initial stages of the drug development process due to their invisible, toxic, and potentially fatal nature. Jamal et al. [17] employed machine learning techniques to unravel the neural networks associated with drugs by integrating biological, chemical, and phenotypic properties to predict ADRs. Similarly, Xue et al used biomedical network topography along the DL domain to infer drug-drug interactions.

Ongoing Pharmaceutical Exploration Projects Utilize AI

Exscientia and oxford - february 2021

Exscientia Centaur is a chemical AI design platform. In Alzheimer's research, The Oxford Institute of Medicine has teamed up with Exscientia to create potential drug candidates for Alzheimer's Disease. In Alzheimer's disease, receptor protein 3 is important for the inflammatory pathway [31].

Insitro and Bristol myers squibb - October 2020

Bristol has teamed up with insitro to develop treatments for neurodegenerative disorder .Insitro a AI driven pharmaceutical exploration development firm has collaborated with Bristol myers squibb .

Genesis therapeutics and Genentech – October 2020

Genetech has cooperated with the biotech company Genentech. This partnership leverages Genetech's therapeutic graphics engine and expertise in pharmaceutical exploration to discover novel drug candidates targeting a wide range of diseases.

Recursion pharmaceuticals and bayer - September 2020

Bayer, a company headquartered in Germany, has entered a collaboration with Recursion Pharmaceuticals, a company based in the United States. This collaboration is using developed new drug candidates for fibrotic disease of lungs and kidneys.

Exscientia and Bayer – January 2020

They are working together to recognise and develop drug candidates for treatment of cardiovascular disease.Exscientia is using AI platform Centaur chemist for this intent [32].

CHALLENGES

In spite of advances in AI algorithms technologies inact in pharmaceutical industry ,there are quiet numerous challenges with regard to performance and combination of these technology into the pharmaceutical exploration and development process.One problem is with unskilled data incorporation This problem arise due to diversity lie between datasets which consist of raw data ,procesed data .proper data collection must be in pharmaceutical exploration process otherwise the machine learning algorithm will be inaccurate . Most suitable method for data incorporation is data banks prior the pharmaceutical exploration process is start.

Another problem is many people do not have the necessary skills to handle AI systems. Third problem is doubt about implementing AI algorithms which is known as black box phenomenon and a deficit of faith for the result generated. All problems lead to slower and less systematic research and development compared with its potential.[33].

DISCUSSION

The integration of artificial intelligence (AI) into drug discovery processes raises significant ethical concerns that necessitate careful consideration. Key areas of focus include ensuring data privacy by adhering to stringent regulations and implementing robust encryption and anonymization techniques to protect sensitive patient information. Additionally, mitigating algorithm bias requires careful curation and validation of datasets to ensure inclusivity and accuracy. Ethical oversight committees must also ensure that AI-generated insights in clinical trials prioritize patient safety, adhere to ethical standards, and respect participant autonomy. While AI holds immense potential to enhance efficiency and accuracy in drug discovery, addressing these ethical considerations is essential to promote responsible and equitable use of AI in advancing pharmaceutical research and healthcare.

CONCLUSION

Regardless the field remaining developing, AI navigate health interventions could show to better health result in low and middle wages countries due to its low price under defined countries. The information provided in this stance and by the profusion of research base outlets, numerous chances subsist now for expansion of innovative estimation methods algorithmic tools that generate degree of cybernation and upgrade the effectiveness of molecules in the drug configuration process. The improvement of AI, along its astonishing tools of spectral analysis, aim to decrease to dare challenges faced by pharmaceutical companies. By integrating AI into drug manufacturing, it becomes possible to customize drugs according to individual preferences, including optimal dosage, release parameters, and other essential properties, thereby offering personalized medication. The capacity of AI to extract critical information has determined the recent vitality in computer-aided drug design, advancing the pharmaceutical exploration process. Present time many pharmaceutical companies facing cost and efficiency issues. There are lot of AI method which make pharmaceutical exploration process cost effective and time efficient.

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