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# Revolutionizing Drug Discovery: The Role of Artificial Intelligence in Modern Pharmaceutical Research

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**Abstract:**

Artificial intelligence, in the recent world is a powerful tool which has been extensively been used scientists working in pharmaceutical industries for drug discovery. Many aspects of drug discovery such as drug screening, identification of dosage, drug effectiveness, virtual screening, QSAR modelling, toxicity prediction, bioactivity prediction, prediction of physiochemical properties, de novo drug design and identification of molecular pathway which were traditionally been time and resource consuming with question of effectiveness has now become less time and resource consuming with remarkable increase in efficiency of the process. The use of different AI tools such as machine learning and deep learning algorithms, DeepAffinity, PREDICT, FAME, XenoSite, eToxPred, pkCMS, wideDTA, DeepChem were found very efficient in analysing huge pool of data and to provide us with most appropriate data use in any process of drug discovery. Several breakthroughs have been achieved in different aspects of drug designing by different scientists resulting in rapid advancement is the field of drug designing.

**Keywords:** Artificial Intelligence, QSAR modelling, Drug discovery, Clinical Trials

## Introduction:

Drug discovery is a very comprehensive process which involves the identification and development of new drug in order to either curing a newly discovered disease or to find out for a better and physiologically more friendly drug to substitute with the existing drug that may cause any adverse or side effect to human body. The process involves several steps such as Target Identification and Validation where a team of researchers identifies the biomolecules that plays an important role in causing the disease to be cure, these biomolecules are then confirmed through methods like CRISPR and RNA interferences, Hit discovery phase where the potential chemical compound are identified through various sources and are identified by using high throughput screening or computational techniques in order to test the vast pool of potential compounds and Hit-to-lead optimization where the selected potential drug is tested for its physiological effect on human body such as efficacy, safety and any side effect and later the potential drug passe through several phase of clinical development in order to be available in the market as a drug.

Drug discovery is a complex, multi-step process involving various stages of research and development aimed at identifying new therapeutic agents. Below is an analytical overview of the key steps involved in drug discovery:

*1.Target Identification and Validation:* -This initial step involves identifying biological targets (usually proteins or genes) associated with a particular disease. After the identification of potential targets, validation of relevance in disease mechanisms and therapeutic potential is required often by conducting molecular and cellular studies [1].

*2. Lead Compound Discovery:* - Following validation of the target identified, lead compounds interacting with that target are screened. With the approach of HTS, virtual screening, and fragment-based drug design, molecules that will show desired biological activity are commonly identified [2].

*3. Lead Optimization:* - The chemical structure of lead compounds is optimized to enhance their efficacy, selectivity, and pharmacokinetic properties (absorption, distribution, metabolism, and excretion). SAR studies guide the optimization process by correlating chemical modifications with biological activity [3].

*4. Preclinical Testing:* - Lead candidates are subjected to rigorous preclinical testing before advancing to human trials to evaluate their safety and efficacy through in vitro (test tube) and in vivo (animal) studies. Also, during this stage, there is a pharmacodynamics assessment of how the drug affects the body and pharmacokinetics of how the body affects the drug.

*5. Clinical Trials:* - The drug then undergoes clinical trials when preclinical tests are quite successful; these clinical trials occur in three phases:

- Phase I: The study is carried out on a few healthy volunteers to assess the safety and dosage [4].

- Phase II: Testing on more patients to determine whether the drug is useful and what side effects it presents [5].

-Phase III: Large numbers of participants to ascertain the drug's efficacy, side effects, and its superiority over standard treatments. Completion of these phases will determine whether or not the regulatory body approves the drug.

*6. Regulatory Review and Approval:* -After successful clinical trials, an NDA is submitted to regulatory bodies. The drugs have all previous study data, manufacturing information, labelling, and suggested use within the application submitted for approval. Agencies scrutinize all applications and permit commercial usage after approval.

*7. Post Marketing Surveillance:* - After commercial use, ongoing monitoring is the need of time in order to observe any late appearing or late appearing side effect not seen at the time of the clinical trials. This stage allows for ongoing data collection and can result in revisions to usage recommendations or additional research.

*8. Market Launch and Commercialization:* - The last step includes strategic marketing and sales activities to promote the drug, which would ensure it is delivered to the target population. Companies must also address patent law and intellectual property rights to safeguard their discoveries.Drug discovery represents a multidisciplinary blend of knowledge from biology, chemistry, pharmacology, and regulatory sciences [6]. Each step is crucial to ensure that new therapies are safe, effective, and good for patients [7]. It takes many years and significant financial investment, which underlines the complexity and importance of the pharmaceutical development pipeline [8].

Traditionally the process was performed only through limited past knowledge and availability of resources and database which limits the reach of the researchers when they are dealing with a new disease [9]. Also, the entire process become too expensive with the estimation of average 2.6 billion US dollars being used in discovery of a single drug along with the average time consumption in the process and launching of drug being

10 years. Still, the success rate of discovery and launching of drug remains less than 10% leading to the risk of wasting of a large number of resources and time [10].

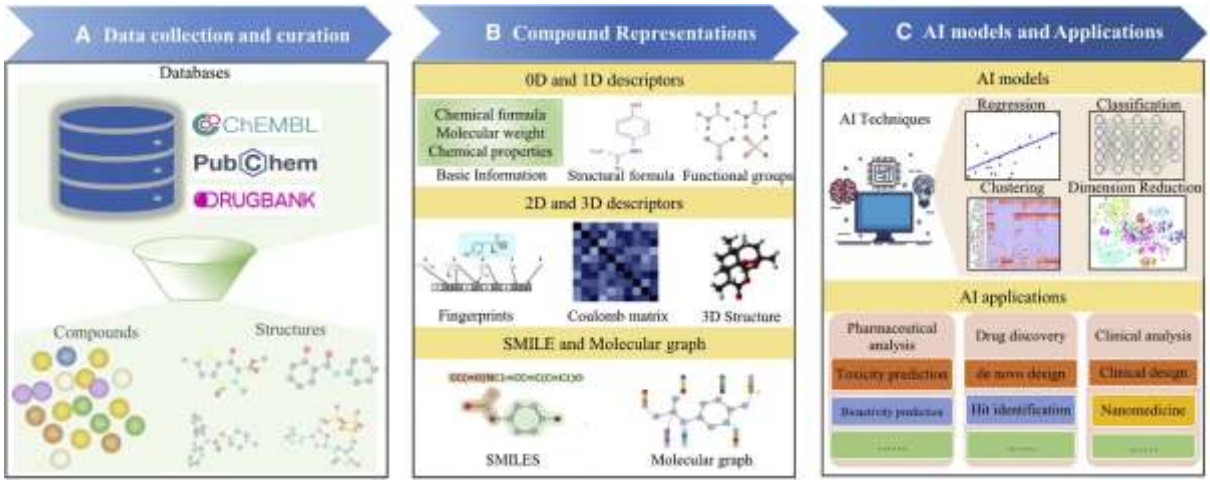


*Figure1. The drug discovery process utilizing AI tools.*

With the advancement of time and technology various new tool are now being implemented in the complex process of drug discovery in order to reduce the consumption of time and resources [11]. Artificial Intelligence have now gained an immense popularity in different fields of research and development, hence now a days is extensively used in the field of drug discovery and development [12]. The vast pool of chemical molecules comprising of approximately $10^{60}$ molecules and still the count is going on earlier use to be a challenge to identify the appropriate set of moieties to work on and to identify the suitable moiety to continue the research, but now with the advancement in artificial intelligence, a vast pool of moiety can be identified and classified according to the requirement. Artificial intelligence had made the complex and time-consuming processes such as hit and trial very time effective and more accurate, also helps in providing the quick validation to the drug target and optimizes the structure designing of drug [13].

**Brief history of drug discovery in AI era:**

Since early 2000s, many machine learning processes such as random forest has been widely been applied for QSAR and VS. in 2012, AlexNet have achieved a remarkable advancement in the deep learning [14]. In same year, Merck Kaggle competition, deep neural networks (DNNs) had shown great performance outperforming the standard RF model in the field of predicting the molecular activity [15]. The recent success of AI in the field of natural language processing and computer vision has provided a great leap in drug discovery process and lead to the great advancement in our deep knowledge of chemistry. In 2019, a great lead was achieved when potent inhibitors of discoidin domain receptor1 (DDR1) were discovered by researchers of Insilico Medicine in only 21 days [16]. In 2020, by the researchers of MIT, halicin, a novel antibiotic candidate against antibiotic-resistant bacteria was identified [17]. It has been noticed that the AI can be greatly used in any stage of drug discovery starting from target identification to determination of drug response in population [18].

**Role of AI in drug screening:**

The process of drug discovery and development takes on an average consumes over a decade with an estimate cost of US$2.8 billion, still only one of the ten therapeutic molecules can pass through the phase II clinical trials and regulatory approvement. A variety of algorithms are now available such as RF, SVMs, Nearest-Neighbour Classifiers and extreme learning machines are used for VS which is based on the synthesis feasibility and also helps in predicting the toxicity and in-vivo activity [19]. Now a days many biopharmaceutical companies such as Pfizer, Roche and Bayer have linked up with many IT companies and working in development of certain platforms which boost up the process of discovery of therapies in the fields such as immuno-oncology and cardiovascular diseases [20].

**Prediction of toxicity:**

It is a vital process in the field of drug development which helps us to identifying the possible toxic effect of the drug in human body by the drug under development [21]. Several web-based tools such as Toxtree, admedSAR, pkCMS are now available to assist the process and reduce both time and money consumption in the process. Advance AI-based approaches are bean now applied for looking similarities among the compounds or to project out the toxicity of compound under development based on the input features [22]. The Tox21 Data Challenge was organized by the National Institute of Health, Environment Protection Agency (EPA) and US Food and Drug Administration (FDA) was an initiation for the evaluation of several computational techniques for forecasting the toxicity of 12,707 environmental compounds and drugs.

SEA was applied for the evaluation of the safety target prediction of 656 drugs in market against 73 unintended markets that might possess the threat of adverse effect on the population [23]. For the estimation of synthetic feasibility and toxicity of small organic molecules, an ML-based approach, eToxPred was applied showing wonderful accuracy of as high as 72% [24]. Other AI open-source tools such as TargeTox and PrOCTOR are being widely used in prediction of toxicity [25]. TargeTox has the ability to produce protein network data and unite the pharmacological and functional properties in a ML classifier for the prediction of the drug toxicity [26]. PrOCTOR is also able to recognize the drugs recognised by FDA which were later reported for showing adverse drug effects [27].

**Prediction of bioactivity:**

The efficiency of drug action in a human body is defined by its ability and efficiency of forming a complex with the appropriate receptors known as drug -receptor complex [28]. Those drug molecules which fails to shows affinity towards the receptors and fail to form drug-receptor complex also fails to show any therapeutic action [29]. This may also lead to interaction of the drug molecule to interact with unwanted protein or receptors leading to unwanted action or even toxicity [30]. Therefore, the drug-target binding affinity (DBTA) plays an important role in predicting the drug-target interaction actions [31]. AI based methods are now widely being used for measuring the binding affinity of the drug molecule to the targeted receptors by comparing either structure similarity or features of both [32]. In interaction based on similarities, the similarities between the drug molecule and target receptor are considered, it has been assumed that similar drugs may bind with the same target receptors [33].

Web applications such as the similarity ensemble approach (SEA) and ChemMapper are been widely been used in recent times for prediction of drug-receptor affinity [34]. Many strategies which involve ML and DL has been widely been used for determination of DBTA such as SimBoost, PADME, KronRLS and DeepDTA.

ML based approach such as Kronecker-regularized least squares (KronRLS) works on the evaluation of the similarities in between drug and protein molecule for determination of DBTA. SimBoost utilizes regression trees for predicting DBTA and mtakes consideration of both the similarity-based and feature-based interactions.

DL approaches, in recent days have shown improvements in performing in comparison of ML because of the application of network-based methods which are independent of availability of 3D protein structure [35]. DeepAffinity, DeepDTA, PADME,WideDTA are some of the widely used DL method has been used for measuring DBTA [36]. WideDTA is CVNN DL method which incorporates ligand SMILES (LS), amino acid sequences, LMCS and protein domains for assessment of the binding affinity [37].

DeepAfffinity is an interpretable DL model which utilizes both RNN and CNN and both the labelled and unlabelled data [38]. PADME is a DL based platform which utilizes feed-forward neural network for the prediction of drug target interactions (DTIs) [39]. Unsupervised ML techniques such as PREDICT and MANTRA are being used for forecasting the therapeutic efficiency of drugs and target proteins for known and unknown pharmaceuticals that can also be extrapolated for the application of drug repurposing and for interpretation of the molecule mechanism of the therapeutics under observation.

**Prediction of physicochemical properties:**

Many physicochemical propertied of the drugs such as partition coefficient, solubility, degree of ionization, and intrinsic permeability of drug causes indirect effect on the pharmacokinetically properties, and the target receptor family, hence must be taken under consideration while developing a new drug. Different AI based tools are now being used for the prediction of physicochemical properties [40]. ML utilizes a large data set produced during the optimization of the compound, previously done for training the program [41]. Algorithms which are been use for drug design includes molecular descriptor, such as SMILES strings, potential energy measurements, coordinates of atoms in 3D and electron density around the molecule for generation of feasible molecules via DNN and hence predict the properties [42].

Zang *et a.* has created a quantitative structure-property relationship (QSPR) workflow for determination of the six physicochemical properties of environmental chemicals obtained from the Environmental Protection Agency (EPC) known as Estimation Program Interface (EPI) Suite. Dl methods such as undirected graph recursive neural networks and graph-based conventional neural networks (CVNN) has been widely been used for the prediction of solubility of the molecular drug [43].

ANN-based models, kernel ridge-based models and graph kernels has been developed for predicting the acid dissociation constant of the given molecule [44]. Cell lines such as Madin-Darby canine kidney cells and human colon adenocarcinoma (Caco-2) cells has generally utilized for generating cellular permeability data of a diverse class of molecules which are been use for AI assisted predictors [45].

**Role of AI in primary and secondary drug screening:**

AI has gradually become a major successful and demanding tool for drug screening due to its ability of processing large number of given information efficiently and in a very small period of time [46]. Certain process like cell classification, cell storing, synthesizing organic compound, developing assay, calculating properties of molecules under study, predicting the possible 3D structure of target molecule are being some of the time-consuming process which have been assisted by AI technology [47]. The process of primary drug screening including the proper classification and shorting of the cell through image analysis has been performed through the use of AI technology [48]. Many ML methods are been used which works on using different algorithms for recognizing images with great accuracy, though showing incompetence while analysing big data [49]. For classifying the target cells, the ML method is needed to be trained for identifying the cell and its features which can be achieve through contrasting the image of the target cells which got separated from the background [50]. Images with different texture features like wavelet-based texture features and Tamura texture feature are extracted, which can be further reduced in dimensions through principal component analyses (PCA) [51]. Many studies shows that least-square SVM (LS-SVM) have shown the highest classification accuracy of up to 95.34% [52].

The process of secondary drug screening incudes the analysis of physical properties, bioactivity and toxicity of the molecule [53]. Partition coefficient and melting point are some of the physical properties of molecule which controls the bio-availability of the molecule and are also been essential for designing a new compound [54]. While designing the drug, molecular representation is done using different methods such molecular fingerprinting, simplified molecular-input line-entry system (SMILES) and Coulomb matrices [55]. The resultant data are been used in DNN, which again comprises of two different stages; generative stage and predictive stage [56]. Although both the stages have been trained separately using supervised learning, when they are trained together, bias can be applied to the output, where it can be either rewarded or penalized for the specific property. Matched molecular pair (MMP) have been widely been used for QSAR studies. MMP has been associated with a single change in drug candidate which have been use for further influencing the bioactivity of the molecule [57]. Now, it has been observed that DNN has the ability to predict better than GBM and RF [58]. With the recent increment in databases, which are easily available to pubic such as ChEMBL, PubChem, ZINC, we have access of a great number of compounds annotating information like

their structure, known targets and purchase ability; MMP plus ML can be used to predict the bioactivity like oral exposure, intrinsic clearance, ADMET and method of action.

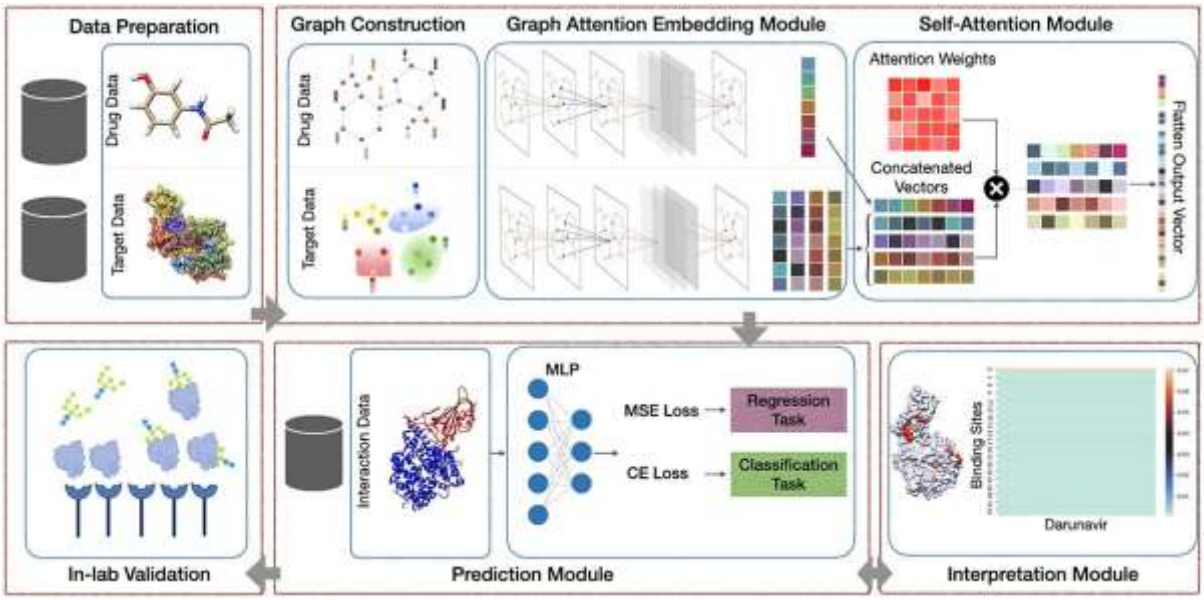


*Figure2. AI based screening model for drug discovery*

**Role of AI in identification of drug dosage and drug delivery effectiveness:**

It is very crucial to properly determine the appropriate dose of any drug to be administered to the patient as improper dosing may lead to improper or unwanted pharmacological action in human body. With the emerge of powerful AI tools, ML and DL algorithms are now been widely used for determining the appropriate dose [59]. Shen *et al.* had developed an AI based platform referred to as AI-PRS which has been use for determination of optimum dosage and combination of drugs to be use in treatment of HIV through antiretroviral therapy [60]. AI-PRS is a neural network-driven approach which is been use to relate drug combinations and dosage to efficacy with the help of parabolic response curve (PRS) [61].

Pantuck *et al.* has developed CURATE.AI for determination of accurate drug dosage, which analyse the patient's personal data and transform it to CURATE.AI profile for assortation of optimal dosage [62]. A study was performed where a combination of cancer drug enzalutamide and investigation drug ZEN-3694 was administered to a patient who was diagnosed with metastatic castration-resistant prostate cancer [63]. By using CURATE.AI it was found that a 50% lower than initial dose of ZEN-3694 was optimum for achieving desired therapeutic result and arrest the growth of cancer [64].

Julkunen *et al.* has devices a comboFM, a novel ML-driven tool which is use to ascertain the appropriate drug combinations and dosage in pre-clinical studies like cancer cell lines [65]. comboFM is use for determination of appropriate drug combinations and dosing with the use of factorization machines, an ML framework for high-dimensional data analysis [66]. In their studies, while using comboFM , Julkunen *et al.* founds a novel combination of anti-cancer drugs crizotinib and bortezomib, which shows promising efficiency in lymphoma cell line [67].

**Role of AI in structure-based and ligand-based virtual screening:**

VS is considered as one of the most important methods of CADD in drug designing a drug screening [68]. The identification of small chemical compound which binds to a drug target is referred to as VS [69]. VS has been considered as one of the most efficient methods for screening out the promising therapeutic compound from a pool of compounds [70]. There exist two main types of VS, those are structure-based VS (SBVS) and ligand-based VS (LBVS). Comparing both the types of VS, SBVS shows a higher accuracy and precision as compared to LBVS [71]. However, recent studied shows that SBVS shows the problem of an increasing number of disease-causing protein and their complicated conformations [72]. For the application of ML in VS, it is to be considered that there must be a filtered training set which comprises of known active and

inactive compounds [73]. Docking is considered to be the main principle for application in SBVS, where in recent times, several AI and ML based scoring algorithms has been developed such as SVR-Score, CScore, ID-score and NNScore. In same way, many ML and DL methods such as RFs, CNNs, SVMs and shallow neural networks have been formed for prediction of protein-ligand affinity in SBVS. Whereas, LBVS, which consist of several steps and each step can be associated with novel AI and ML based algorithms for speeding up the process and for increasing reliability [74]. Several ML and Dl based algorithms has been build up for preparing useful decoy sets such as Gaussian mixture models (GMMs), isolation forests and artificial neural networks (ANNs) [75]. Further, ML models such as HEX, PARASHIFT, ShaPE and USR algorithms has been developed for LBVS [76].

Liu *et al.* 2017 had discovered low toxicity O-GlcNAc transferase inhibitors, Dou *et al.* have identified novel glycogen synthase kinase 3 beta inhibitors by using SBVS. Gahlawat *et al.* 2020 has identified that saquinavir, lithospermic acid and 11m_32045235 were found to be promising therapeutic compound against SARS-Cov-2 main proteas. Selvaraj et al. 2020 demonstrated that TCM 57025, TCM 3495, TCM 5376, TCM 20111, and TCM 31007 were those therapeutic compounds which interacts with the substrate-binding site of N7-MTase [77]. Cruz *et al.* 2018 concluded that ZINC91881108 was a potent compound against RIPK2 [78].

**Role of AI in QSAR modelling:**

Quantitative structure–activity relationship (QSAR) modelling seeks to establish a connection between the various properties and activities of different chemical compounds and their corresponding molecular structures [79]. As the dataset, which includes numerous compounds that possess quantitative values along with detailed molecular structural data, continues to expand significantly, it becomes increasingly important to develop a rapid and effective large-scale screening technology. This technology will be essential for efficiently selecting and accurately identifying those chemicals that demonstrate high activity levels [80]. R modelling has become an increasingly popular method [81]. Over four decades, QSAR models have been used substantially in the drug, environmental, material, food, and other chemical domains [82]. Therefore, the search for more efficient, practical, and accurate methods for establishing QSAR models and predicting activities has become necessary [83]. The recent proliferation of cyber infrastructure, availability of extensive public domain and proprietary databases, coupled with advancements in cheminformatics and molecular descriptors, has created a terrific impetus to apply machi SAR-type predictive tasks especially in Q SAR-type.

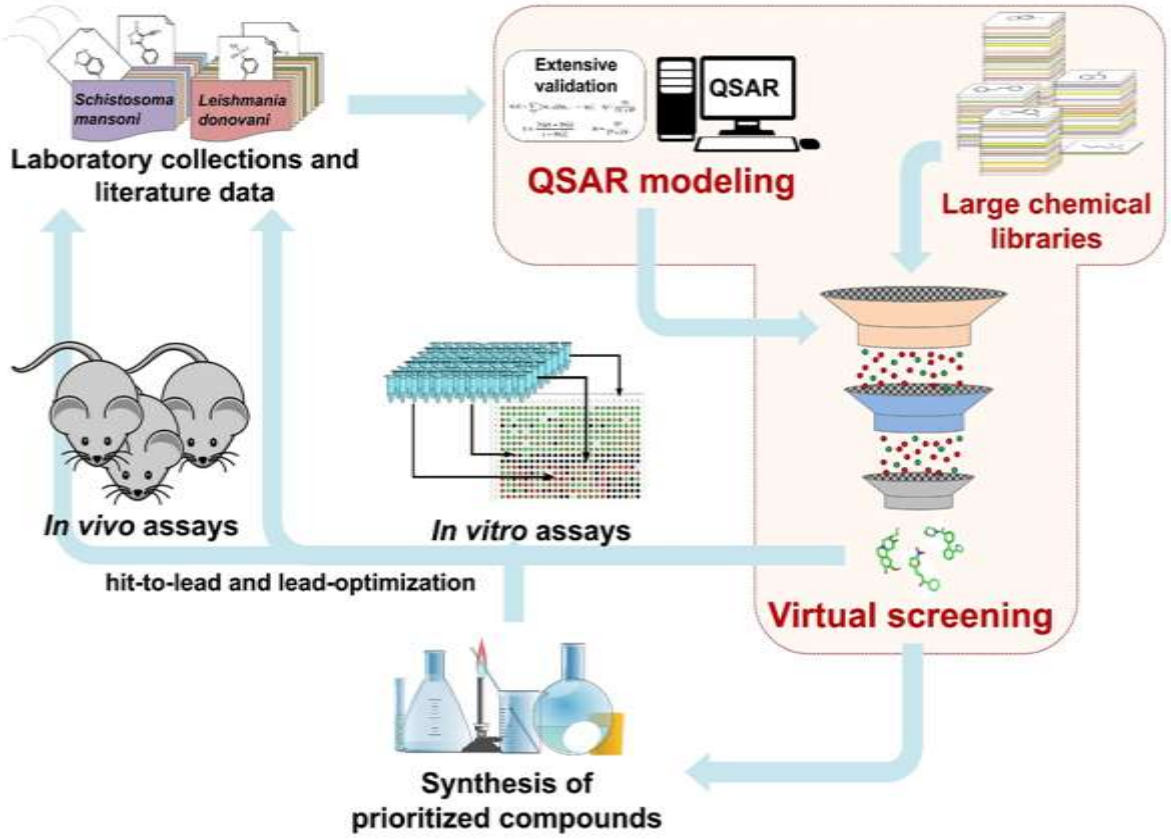


Figure3. Application of QSAR modelling in drug discovery.

The traditional methods of QSAR modelling mainly focus on multiple linear regression analysis, which is a simple and useful method [84]. However, this method has certain limitations. For example, the correlations derived with this method lack clear cause-and-effect relationships [85]. It is difficult to identify the most important physical, chemical, or biological features based on the correlation results [86]. Moreover, the nature and type of the responses that can be predicted are greatly restricted. In addition to the shortcomings of multiple linear regression analysis, the high dimensionality of the molecular structural features will bring serious problems to the data processing in the traditional QSAR models [87]. As a result, dimensionality reduction becomes a priority problem. In summary, in a broad class of chemical, biological, and structural domains, much high-dimensional data makes drug and chemical property prediction difficult using traditional methods [88]. With the rapid development of neural network technology and the wide application of neural networks in many other domains such as voice recognition, image recognition, and so on, people have also started gradually to apply artificial neural networks to QSAR modelling.

The recent advancement and increase in application in application of ML algorithms such as neural networks, SVM and DL has supplied with a greater avenue for QSAR modelling [89]. Many web-based tools and algorithms have been recently been developed for QSAR modelling like VEGA platform, QSAR-Co, FL-QSAR, Meta-QSAR, DPubChem, Transformer-CNN, Cloud 3D-QSAR, MoDeSuS and Chemception [90]. *Karpov et al*. 2020 developed a novel algorithm for QSAR modelling which is based on ANN known as transformer-CNN. *Wang et al*. 2020 developed QSAR modelling web-based tool with intregation of characteristic features of modelling structure generation, alignment and molecular interaction field [91]. *Jin et al.* with the help of Cloud 3D-QSAR discovered a potent and selective monoamine oxidase B (MAO-B) inhibitor. *Bennett et al.* 2020 with help of Chemception, has predicted the small molecules transfer free energy with combination of MD stimulation and DL.

**Role of AI in de novo drug designing:**

The drug design process, as the name itself indicates, is a process of finding a compound that can treat a disease [92]. That drug compound has biochemical effects on the signalling pathways related to the disease [93]. Drug design techniques combine knowledge of biochemical pathways and the response of living beings to chemical compounds [94]. The drug designing pipeline is a very complex framework. Finding an active compound through experimental procedures is tricky and has delays [95]. Hence, in silico methods have emerged as fast but cheaper methods for reducing the time of drug discovery [96]. De novo drug designing is a computational method where the fabrication of a new drug is automated and a suitable lead compound is found [97]. This eliminates the need for a brute force evaluation of large libraries of compounds. The drug discovery process involves the identification of a target, validation of the target, finding initial hits, lead optimization, and clinical testing [98]. De novo drug designing can significantly reduce the time needed for the lead generation stage of the above workflow [99]. The core idea of de novo designing is that we can build efficient models of candidate compounds, given a library of available building blocks, and then select the models that are expected to possess the most favourable drug-like properties [100]. Computer-aided drug design tools assist in all steps, specifically in guiding the design of novel drugs that are backed by the principles of medicinal chemistry [101]. The current work presents how AI is leveraged in de novo drug designing, also discussing the use of graph neural networks for the design of new molecules [102].

RNN has been likely found effective for utilizing in de novo drug design [103]. As the SMILES strings has encoded the substance structure in a grouping of letters, RNN has recently been utilized for generating compound structure [104]. It was found that RNNs have shown a great potential for utilizing SMILES strings for drug design [105]. Optimizing AI and multi-objective has been seen as a promising solution for bridging the chemical and biological phase [106]. Novel pairs of multi-objectives based on RNN for the automatization of de novo drug design based on SMILES has been developed for finding the best possible match between physicochemical properties and their constrain biological targets. ML models like SVM, DNNs and RF and many others have recently been widely used for drug discovery and for analysing the pharmaceutical applications from docking to VS [107]. The first de novo multi-target drug configuration program called LigBuilder V3 has been developed to design the ligands for different receptors, numerous coupling locales of one receptor or various configurations of one receptor [108]. LigBuilder has been again used for multi-target drug plans and enhancements, especially for compact ligand of proteins with different ligand binding sites [109]. Fragment-based de novo design tools were successfully found applicable in discovering non-covalent inhibitor [110]. A new protocol, known as Cov_FB3D has been developed that involves the in-silico assembly of potential novel covalent inhibitors by identification of the active fragments in the covalently binding site of target protein [111].

**Role of AI in identification of molecular pathway:**

Molecular pathways represent a sequence of interactions between different molecules inside cells and in-between cells that are needed to accomplish one or more functions [112]. Therefore, the identification and thorough understanding of these complex series of interactions is of fundamental importance in molecular biology, and key for associating molecular observations with phenotypes [113]. Here, we discuss and overview a variety of current research that utilizes Artificial Intelligence models to identify and evaluate these complex cellular pathways. The AI models presented in this research range from more traditional approaches such as sequence-based support vector machines or the random forest models to contemporary deep learning models [114]. We start by introducing the need for molecular pathway identification before describing the various types of methods that have been employed to create these hot-topic models [115]. The fundamental biological unit in the functional aspect is the pathway, yet defining pathway activity is not as straightforward as defining gene or protein activity [116]. The number of matched gene-expression data termed as pathway activity is zero if no genes are differentially expressed or significant matching is not achieved by chance [117]. The level of expression of the genes, the actual presence of the gene products in the cells and the amount present, as well as gene expression, similarity can be caused by mutations and gene transfer events [118].

Interpretation of the relationship between the abundance of the molecule measured by microarrays and the biological events taking place in this process involves the identification of biological pathways associated with this data [119]. Indeed, describing gene function rather than gene-level data can greatly enhance our understanding of biological processes. Because with the known data, researches focus on clustering views instead of gene-level views.

The recent advancement in AI tools in the field of drug discovery and development has led to development of various web-based tools and stand-alone software packages for polypharmacology predictions like polypharmacology browser (PPB), TarPred, Self Organizing Map Based Prediction of Drug Equivalence Relationship (SPiDER), Targethunter, PharmMapper, ChemMapper and Swiss Target Prediction (SwissTargetPrediction). *Poirier et al.* 2018 conducted an experiment with the help of PPB for identifying lysophosphatidic acid acyltransferase beta as a therapeutic target of nanomolar angiogenesis [120]. *Ozhathil et al.* 2018 identified potent and selective small molecule inhibitors of cation channel transient receptor potential cation channel subfamily M member 4 with the help of PPB. Vleet Van *et al.* 2018 applied TarPred tool for screening strategies and methods for improved off-target liability prediction [121]. Ratnawati *et al.* predicted the active compound from SMILES codes by using backpropagation algorithms [122]. OpenTargets, a ML-based and freeware tool was used to priotize potential therapeutic drug targets with the accuracy of over 71% [123]. Nabirotchkin *et al.* identified unfolded protein response and autophagy-related pathways for the drugs commonly been approved against COVID-19 [124]. Lopez-Cortes *et al.* identified allele frequencies in colorectal cancer.

**Conclusion:**

The advancement of AI and the tools associated with it has proven to be boon to pharmaceutical industries with their remarkable contribution in many steps of drug discovery like target identification, QSAR modelling, comparison of physiochemical properties of molecule, primary and secondary drug screening. The tools have made the process faster and more accurate with less consumption of both time and resources. In recent years, many drugs were discovered in recorded time during crises like Ebola epidermic and COVID pandemic resulting in saving lives of millions. The recent collaboration of many IT companies with pharmaceutical industries in developing new and more powerful AI tools also shows the revolutionary acceptance of AI technologies resulting in advancement in traditional drug discovery process.

Though, a major problem has evolved in pharmaceutical industries around AI is that there is a worldwide shortage has been observed in skilled personalities able to handle the latest AI tools. This also led to an upcoming crisis of loss of employment of traditional working force who have no knowledge of using recently developed AI tools and are unable to co-operate with the rapid change in industry. For tackling such upcoming problems, it is required to teach the upcoming work force with the proper knowledge of AI tools in institutions along with appropriate practical knowledge and the current working force is also needed to be train with collaboration of professionals of the field by conducting appropriate seminars and workshops so that they can also remain a crucial part of this rapidly modifying industry.

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