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Research

THE EXPANDING ROLE OF ARTIFICIAL INTELLIGENCE IN MODERN DRUG DEVELOPMENT

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Abstract

In pharmaceutical research, artificial intelligence (AI) has emerged as a transformative tool that tackles persistent issues like high development costs, protracted timetables, and low clinical success rates. AI speeds up several phases of drug development, including target identification, virtual screening, hit-to-lead optimisation, preclinical evaluation, and clinical trial design, through the integration of machine learning (ML), deep learning (DL), and advanced computational models. Prediction accuracy for protein structures, drug-target interactions, toxicity profiles, and ADMET attributes is improved by contemporary AI technologies like AlphaFold, DeepChem, Atomwise, and generative models like GANs and RNNs. De novo molecular design and AI-driven virtual screening make it possible to quickly find new candidates with enhanced drug-like characteristics. Additionally, adaptive clinical trial systems, phenotype-based screening, and AI-based digital twins greatly increase clinical success. AI continues to influence the future of pharmaceutical manufacturing, nanomedicine, and personalised medicine despite issues with data quality, transparency, and interaction with conventional workflows. When taken as a whole, AI provides a scalable, economical, and effective framework that is revolutionising innovation in contemporary drug research and discovery. AI continues to transform pharmaceutical research and personalised treatment in spite of obstacles like data quality, openness, and regulatory concerns.

Keywords: Artificial intelligence; Machine learning; Deep learning; Drug discovery; Drug development; Virtual screening; ADMET prediction; Target identification; De novo drug design; Clinical trials; Computational pharmacology; Pharmaceutical innovation.

INTRODUCTION

The process of finding a new medication is difficult, costly, and prone to failure. The average cost of developing a new medication is about $2.5 billion, and the process can take more than ten years [1]. Furthermore, only a tiny percentage of medication candidates that start clinical trials are ever approved by regulators [2]. In spite of the efforts, only 2.01% of a successful, commercially viable medication is the end product of drug development initiatives [3]. Significant barriers in traditional drug discovery and development contribute to their high costs, long schedules, and frequent failures. These obstacles include the resource-intensive nature of high-throughput screening for lead compounds; the time-consuming and tedious process of finding viable pharmacological targets; iterative and costly optimisation of lead drugs to improve safety, efficacy, and selectivity; and the difficulties associated with planning and conducting processes effective clinical trials, including as patient recruitment, data collecting, and analysis.[4] Drug development firms have used a variety of strategies to get around this problem, with artificial intelligence (AI) being crucial. For instance, a study conducted by the technology company Tech Emergence found that using AI to develop new drugs can accelerate the process by 2%, and a Goldman Sachs report estimated that as AI technology advances, the potential annual savings in this area are estimated to reach 28 billion dollars .[5]

TECHNOLOGY AND ALGORIITHM RELATED IN DRUG DISCOVERY AND DEVELOPMENT

Deep learning (DL) is a subset of machine learning (ML), which is a branch of artificial intelligence (AI) .[6] AI is currently capable of performing DL and analysing more complicated algorithms. Numerous For the purpose of drug development, similar computational models have been created. Peptide synthesis, structure-based virtual screening, ligand-based virtual screening, toxicity prediction, drug monitoring and release, pharmacodynamic modelling, quantitative structure-activity relationships, drug repositioning, polypharmacology, and physicochemical activities are just a few of the drug discovery processes that have made use of machine learning algorithms .[7]

MACHINE LEARNING

Machine learning (ML) is the term for AI algorithms that use massive datasets to train models in order to learn rules, analyse fresh data, and make predictions and decisions. Three primary categories of ML exist: supervised education, Reinforcement learning and unsupervised learning.[8] In order to accurately anticipate new, unknown inputs, supervised learning entails training algorithms using labelled datasets with preset correct answers for each input. [9]With results like illness subtypes and target identification,(fig:1). For example, Chen et al. assembled 148,784 transcripts and 78,092 single genes from clean readings using the Trinity software.
[10,11]

MACHINE LEARNING ALGORITHMS

The most popular machine learning algorithms used in drug research and discovery are Random Forest (RF), Support Vector Machine (SVM), Naïve Bayesian Classifier (NB), and kNearest Neighbours (kNN) and ANNs (Artificial Neural Networks) .The following is a summary of their contributions to drug development and discovery.

K- NEAREST NUMBER (KNN)

A sample is assumed to fall into a certain category if the majority of the k-nearest samples (the closest neighbours in the feature space) that surround it fall into that group [12]. In order to increase the overall density of the medication-disease association matrix based on the kNN principle for drug repositioning research, Yang M et al. recently employed the weighted kNN (WkNN) technique .[13]

NAIVE BAYESIAN CLASSIFIER (NB)

Naive Bayesian classifier that can be used to train a model using a dataset of known categories is NB, which makes it possible to classify data from unknown categories . [14]The pharmaceutical industry has employed NB because of its ease of use, efficiency, and speed. For example, Shi H et al. trained a classifier to identify positive and negative samples of the pregnane X receptor (PXR) using the NB principle. The classification efficiency was then increased by using this classifier to differentiate between PXR activators and non-activators [15]

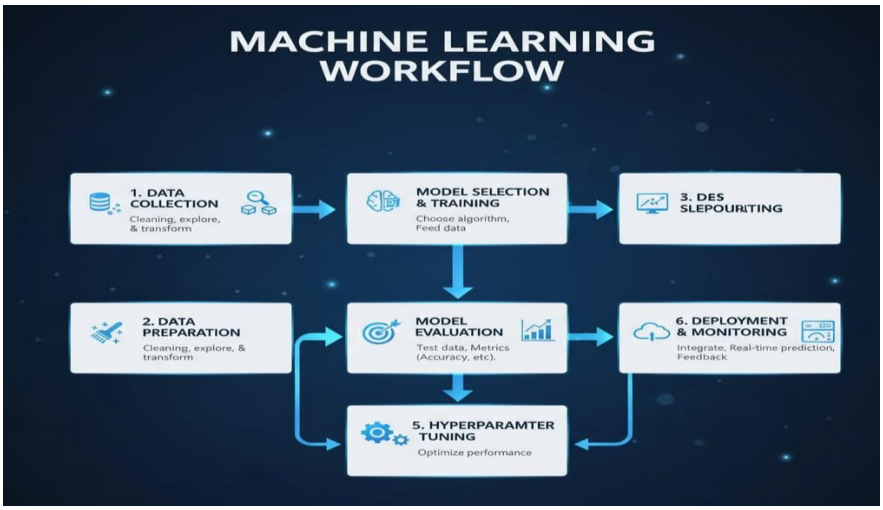

Figure 1: Machine Learning Work Flow

RANDOM FOREST (RF)

RF is an ensemble or group of Classification and Regression Trees (CART) [16] that have been trained on datasets that are the same size as the training set bootstraps, which are produced by randomly resampling the training data. After a tree is built, a set of bootstraps—also known as out-of-bag (OOB) samples—that do not contain any specific record from the original dataset are used as the test set. The OOB estimate of the generalisation error is the classification error rate for each test set. [17]

SUPPORT VECTOR MACHINE (SVM)

A two-class classification model is the SVM. It uses an interval learning approach. maximisation, which in turn means resolving a convex quadratic programming issue Predicting molecular interactions, binding affinity, and other characteristics between ligands and target proteins is essential. [18] Using a web database and a combination of SVM with Cfs subset evaluation and Best First-D1-N5 search, Jing-Fang Z et al. identified 324 neurotoxic compounds and 234 non-neurotoxic compounds. The dataset utilised to build the neurotoxicity discriminant model was compounds. [19]

ARTIFICIAL NEURAL NETWORK (ANNs)

Artificial neural networks (ANNs) are computer programs that replicate the functioning of several processing units that resemble nerve cells and the fundamental biological processes by which they communicate and interact with one another. As direct analogues of biological NNs, artificial neural networks (ANNs) are a subset of machine learning. ANNs can learn from experiences and comprehend the broad correlations between variables, just like the human brain.(20)

DEEP LEARNING ALGORITHM

DL algorithms for drug discovery usually consist of convolutional neural networks (CNNs), generative adversarial networks (GANs), and recurrent neural networks (RNNs). All of them play critical role in drug discovery and development, which have been summarized as following.

CONVOLUTIONAL NEURAL NETWORK (CNNs)

Convolutional filters, which are usually tiny matrices of 3 × 3 or 5 × 5 in size, are used by CNNs' convolutional layer to slide over the source image and extract particular features. Consequently, following maximum pooling and average pooling by a pooling layer, there is less computation and a lower chance of overfitting. A completely connected layer receives these as an input after they have been compressed into a lengthwise vector. These characteristics are then used by the fully connected layer to classify images. (21)

GENERATIVE ADVERSARIAL NETWORK (GANs)

A discriminator and a generator are necessary for a GAN to function. The generator generates new samples from random inputs, which are subsequently supplied to the discriminator. To discern between authentic and fraudulent. In order to produce more genuine sample data, these two elements constantly compete with one another (22). For example, a new CNN was built with dense networks. Dense networks expand the training space

and boost sequence generation efficiency by performing multilayer transmission on the GAN architecture's generator network
(23).

RECURRENT NEURAL NETWORK (RNNs)

Due to their capacity to handle images and time series, RNNs are especially crucial for information analysis based on sequences or time series. numerical data and discover data kinds that show forward and backward correlations because of the network's innate capacity to retain them. Sangrak et al. built an RNN model that greatly enhanced drug interaction extraction performance by combining positional characteristics, subtree inclusion features, and integration techniques. This model was based on the benefits of RNNs for data processing.[24]

ARTIFICIAL INTELLIGENCE IN DRUG DICOVERY

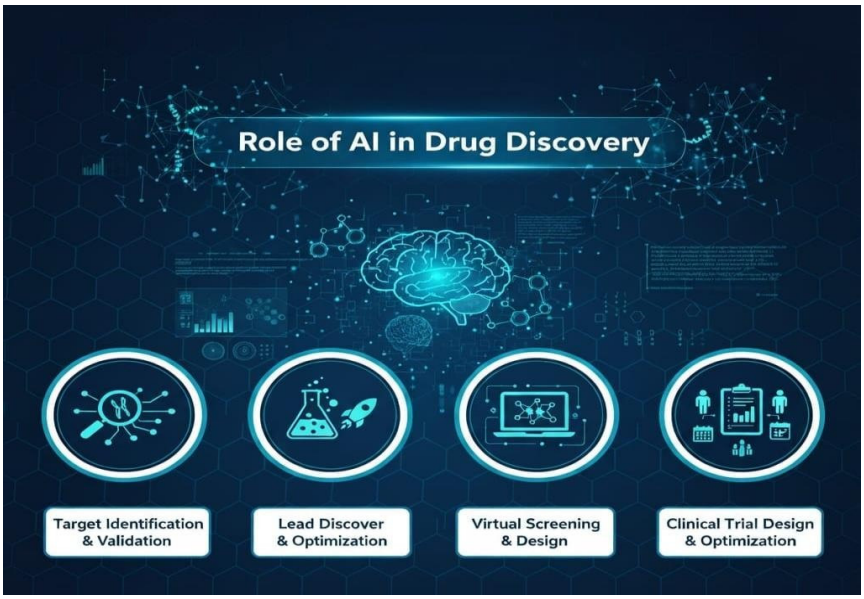

Figure 2: Artificial Intelligence In Drug Discovery

AI IN TARGET IDENTIFICATION

Finding appropriate pharmacological targets is a crucial stage in the drug development process because it defines the molecular mechanisms and biological pathways that can be altered to provide therapeutic effects. Algorithms for machine learning are essential for target identification. These algorithms find possible disease-associated targets and rank them for more research by examining a variety of genomic, proteomic, and clinical data datasets [25]. The abundance of biological data, such as gene expression patterns, protein–protein interaction networks, and illness phenotypes, is one of the primary obstacles in target identification. (figure:2) Machine learning algorithms can uncover hidden relationships between biological entities and identify potential drug targets based on their expression patterns, functional annotations, and disease associations by using dimensionality reduction techniques like principal component analysis (PCA) and t-distributed stochastic neighbour embedding (t-SNE) [26].

Additionally, prospective drug targets can be ranked according to their druggability, safety profiles, and therapeutic relevance using machine learning algorithms that combine data from several sources. In this regard, machine learning is used by the Drug Gene Interaction Database (DGIdb). Algorithms to identify pharmacological targets from known interactions from approved medications and investigational compounds by curating and annotating known drug– gene interactions from various sources [27]. In order to identify possible targets based on their transcriptional fingerprints and functional annotations, the connectivity map (CMAp) also employs machine learning techniques to examine gene expression profiles from drug-treated cells .The connection map was created to close a gap caused by the absence of techniques for methodically figuring out a compound's cellular effects and the unanticipated off-target activities that

would only be found later in the drug's life. Development procedure that can restrict the compound's application in medicine.[28]

AI IN HIT IDENTIFICATION AND VIRTUAL SCREENING

A critical stage in the drug development process is virtual screening, which involves computationally analysing vast chemical libraries to discover molecules with a strong propensity for binding or engage with a particular biological target [29]. The 3D structure of the target is employed in structure-based virtual screening (SBVS) to forecast how various chemicals will attach to the chosen pocket. This technique necessitates a thorough understanding of the molecular interaction site on the target [30]. In the past, docking simulations required creating several molecular postures and calculating the binding energy scores for each ligand-target interaction. Although promising , ML has played a significant role in ligand-based virtual screening (LBVS) techniques, employing the characteristics of previously identified ligands for the particular target of interest . Quantitative StructureActivity Relationship (QSAR) prediction models have been widely used to identify potential drug candidates [31].

The latter is frequently employed in SBVS techniques, which depend on understanding the target protein's three-dimensional structure and substances to screen for candidate molecules with inhibitor activity. In this domain , [32].The creation of new scoring functions is receiving a lot of attention since they can help with further components of drug design, particularly lead compound optimisation, QSAR models, and the prediction of absorption, distribution, metabolism, excretion, and toxicity (ADMET) features. In practice , machine learning approaches have proven to effective better than conventional scoring algorithms [33].

New DL-based scoring algorithms are starting to gain traction for virtual screening tasks ,convolutional neyral network (CNN) models in particular . Large volumes of data may be processed by these models, which can also identify patterns in chemical structures that correspond to successful binding to biological targets. Traditional ML techniques are anticipated to be increasingly replaced by DL scoring functions as more high-quality experimental data becomes publically available. [34]

AI IN VALIDATION PROCESS

Validation is essential to ensuring the therapeutic relevance and efficacy of a putative target after it has been identified. This procedure has historically required a lot of in vitro and in vivo studies, which are expensive and time-consuming. AI has given rise to computational models that mimic biological systems and forecast the consequences of altering a particular target, such as graph neural networks (GNNs) [35]. These models assess how tiny compounds interact with protein targets and how those interactions affect biological circuits.Target-drug interaction prediction has benefited greatly from deep learning algorithms. By reducing the need for lab trials, these computational methods speed up the validation process without sacrificing accuracy.(36)

AI IN LEAD OPTIMIZATION

Lead optimisation uses iterative chemical alterations to enhance the potency, selectivity, and pharmacokinetic characteristics of possible drug candidates. Lead optimisation has historically depended on time-consuming and labour-intensive experimental techniques, such highthroughput screening, which frequently led to expensive failures and less-than-ideal compounds. A more methodical and data-driven approach to lead optimisation is provided by machine learning techniques, which enable increased accuracy and computational efficiency in predictions of the biological activity and drug-like characteristics of novel chemical analogues. The use of machine learning-based lead optimisation enables the prediction of the structure–activity relationships (SARs) underpinning drug-target interactions by learning from extensive databases of molecular architecture and related pharmacological activities. Through instruction Machine learning algorithms can identify molecular features and substructures that contribute to the desired biological effects using predictive models on annotated datasets of known compound activities. This reduces the need for expensive and time-consuming experimental validation and guides logical design decisions. GANs and QSAR modelling have become more common machine learning techniques. In this way, the DeepChem framework use deep learning algorithms to accurately predict the biological activities of novel molecule analogues by directly learning molecular representations from chemical structures [37]. TABLE: 1summary of software platforms that utilize AI techniques,[38]

Table 1

SOFTWARE PLATFORM	DESCRIPTION	KEY FEATURES
DeepMind AlphaFold (Google, Mountain View, CA, USA) https://deepmind.google/technologies/alphafold	Deep learning model for protein structure prediction	Predicts protein structures with high accuracy
Atomwise (Atomwise Inc., San Francisco, CA, USA) https://www.atomwise.com	AI-driven drug discovery platform	Virtual screening, lead optimization
Recursion Pharmaceuticals (Recursion, Salt Lake City, UT, USA) https://www.recursion.com	High throughput screening platform	Cellular phenotypic analysis ,rare disease
Benevolent AI (Benevolent AI, London, UK) https://www.benevolent.com	Drug discovery and development platform	Predictive modelling, target identification
Schrödinger Maestro (Schrödinger, New York, NY, USA) https://www.schrodinger.com	Molecular docking and simulations	Molecular docking, QSAR modelling
XtalPi (Quantum Pharm Inc., Boston, MA, USA) https://www.xtalpi.com	AI-driven drug crystal prediction	Predicts drug crystal forms, stability

AI IN PRECLINICAL AND CLINICAL DEVELOPMENT

The integration of AI and ML into clinical trials is a sophisticated approach that continues to change many aspects of clinical research. From patient recruitment to real-time adaption, predictive modelling, and guaranteeing ethical behaviour, these technologies provide a variety of instruments for speeding up the development of novel medical therapies in a patient-centric manner.[39- 41] AI-driven digital twins can mimic virtual patient populations by predicting treatment results and doing away with the need for massive control groups, leading to quicker and more accurate clinical research. The AI teams working on clinical trial themes include DeepDrug (eMolFrag, eSynth, eToxPred, eDrugRes, eVir, eComb) and Benevolent AI (knowledge graphs and protein pocket analysis). Exscientia had expanded by 2024, and six AI-designed drugs had begun clinical trials. These consist of oncological, psychosocial, and immunological therapy [42] .

CLINICAL TRIAL DESIGN

Another area where AI is having a significant impact is clinical trial design. Clinical trials are usually the most costly and time-consuming stage of drug development, and a number of potential medications are derailed by inadequate patient selection, trial design, or side effects. By evaluating treatment results, locating suitable candidates, and analysing patient data, artificial intelligence improves research endeavours. It is simpler to run studies with patients who are most likely to benefit from the medication when machine learning algorithms are able to classify patient groups based on genetic, clinical, and demographic variables [43]. AI-powered adaptive trial designs can change treatment duration, dose, and even patient enrolment in real time based on outcomes. This Adaptive strategy expedites approval and optimises trial success. Natural Language Processing (NLP) techniques speed up the design and conceptualisation of trials by making it easier to quickly get information from clinical record, medical literature, and other textual sources. AI/ML helps create novel clinical trials by utilising machine learning techniques, data mining, predictive modelling, and natural language processing (NLP) [44] [45] .

PREDICTING THE ABSORPTION, DISTRIBUTION, METABOLISM EXCRETION AND TOXICITY TOLERANCE (ADMET) PROPERTIES OF COMPOUNDS

Strong biological activity, advantageous physicochemical properties, superior ADMET qualities, and effective pharmacokinetic mechanisms. The failure of drug development efforts is largely due to the poor pharmacokinetic properties and possible toxicity of candidate molecules. Drug delivery methods with low levels of immunogenicity and toxicity are essential for measuring the success of targeted interventions in

cancer therapies , a rapidly developing anticancer therapy paradigm .

By examining the chemical structures and characteristics of molecules, AI can be used to forecast the toxicity of drugs.(fig:3) ML algorithms that have been trained on toxicology datasets are able to anticipate negative consequences and recognise dangerous structural characteristics. During clinical studies, this prediction ability helps researchers prioritise safer drugs and minimise negative consequences.

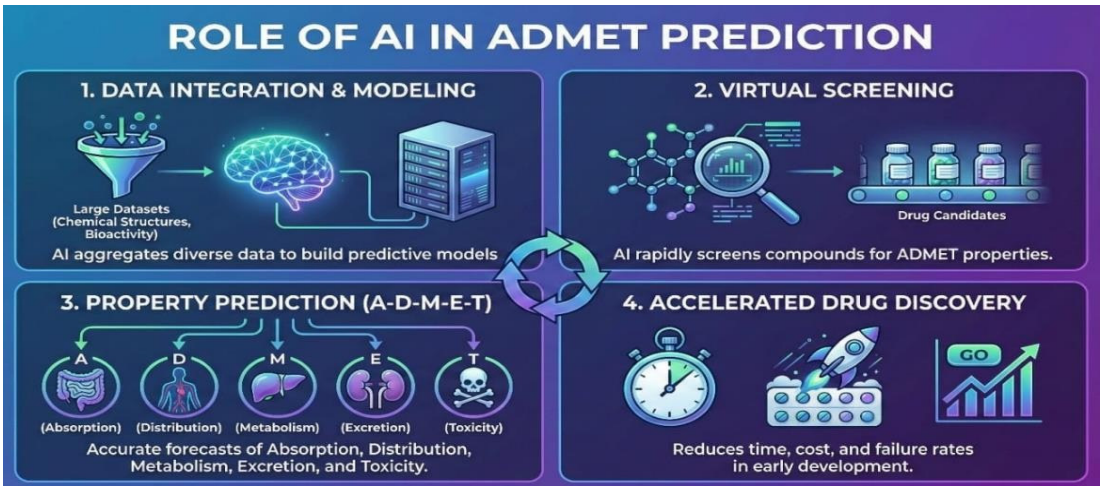

Figure 3: Role of AI In ADMET Prediction

For example, presented the ADMETlab model, which is based on version 2.0 built with the Python Web framework Django and is based on in silico ADMET. With 17 physical chemistry, 13 medicinal chemistry, 23 ADME characterisation, 27 toxicity endpoints, and 8 toxicogenic rules, this model which is hosted on the AliCloud Ubuntu Linux system offers a wider variety of ADMET endpoints than its predecessor.[46]

DE NOVO DESIGN OF BIOACTIVE SMALL MOLECULES BY AI

The goal of computational de novo design is to create novel chemical entities with desirable characteristics. [47] A novel approach to de novo molecular design based on generative artificial intelligence (AI) has just been put forth. It shows potential as a method of learning from known bioactive chemicals and creating new molecules on its own that have inherited synthesizability and bioactivity. [48]

Crucially, it is anticipated that these generative techniques would generate chemically accurate structures without requiring the explicit inclusion of building block libraries or guidelines for their fusion and chemical transformation. Nevertheless, up until now, generative AI has only been used for retroactive de novo design by the replication of known bioactive ligands or generative anticipated actions.

We use generative AI in this first prospective investigation to investigate if it can produce bioactive de novo designs that are truly synthesizable. There were two fundamental steps in the computational technique. Initially, we created a generic model that used a sizable, unfocused compound collection to learn the composition of druglike compounds.

We then improved this general model using more precise chemical characteristics from a small target-focused library of actives. We used a recently published deep recurrent neural network (RNN) with long short-term memory (LSTM) cells for the general model. [49,50]

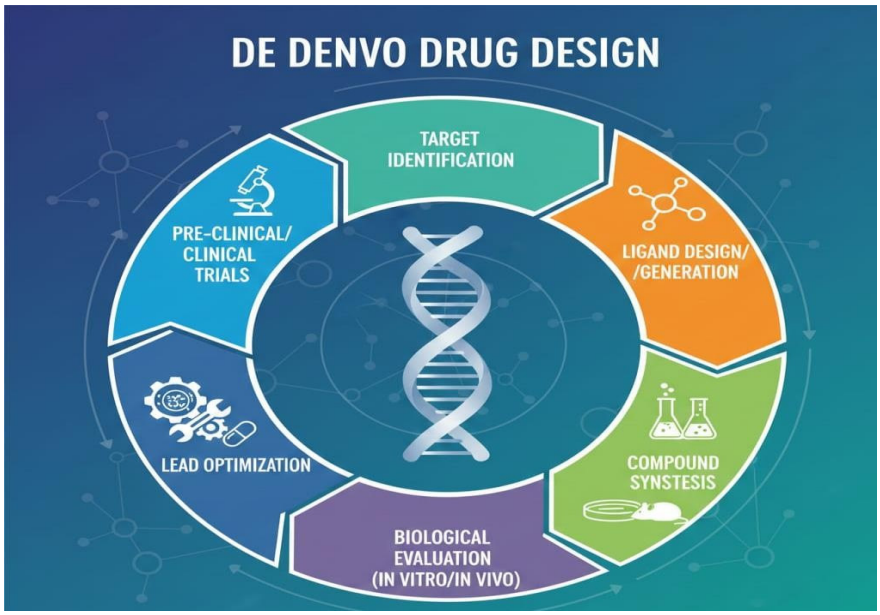

Figure 4: De Novo Drug Design

CASE STUDY

COVID -19

The SARS-CoV-2 coronavirus that triggered the COVID-19 pandemic has brought forth formerly unheard-of worldwide issues in the areas of public health, economics, and society. As of October 2022, the extremely contagious virus had caused over 6.5 million deaths and over 620 million confirmed cases since it first appeared in late 2019.

A promising tool that offers data-driven solutions to major challenges in managing the pandemic is artificial intelligence (AI). Advanced Large-scale datasets pertaining to coronavirus transmission, disease progression, patient outcomes, population movement, and health care operations can be used to uncover insights utilising deep learning and machine learning approaches.

DRUG DEVELOPMENT

Repurposing current medications is essential in the hunt for COVID-19 therapies due to the difficulty of drug design and clinical trials. Mohapatra and colleagues used machine - earning models to a Pub-Chem dataset. They used mathematical classifiers for supervised learning so that the system could learn from datasets with specifics and useful results. It was discovered that the naive Bayes classifier was the best option since it avoided the overfitting problems that random forest or sequential minimum optimisation algorithms had.

The model's medication prediction accuracy was about 73%. In the end, they concluded that amprenavir, an antiretroviral medication, was the most successful in combating COVID-19 infection. To find possible candidates for medication repurposing, researchers have performed drug-based prediction of antiviral activity against COVID-19. Using in vitro data encoded with chemical fingerprints that represent certain molecular substructures, Delijewski and Haneczok created a supervised machine learning model.

A crucial step in identifying drug effects and carrying out drug repurposing is investigating drug–target interactions (DTIs). A DTI prediction model that particularly incorporates protein sequence and structured data was presented by El-Behery et al. The model employs encoding approaches to extract features based on the physical and chemical characteristics of protein amino acid sequences. SMILES (Simplified Molecular Input Line Entry System) medication strings. The interactions between medications and target proteins in human cells are then predicted using a variety of machine learning, deep learning, and ensemble learning techniques. They found possible medications that might be repurposed by exploiting proteins impacted by COVID-19 infection in human cells. For instance, they estimated that the ACE2 protein would interact with DB00691 and DB05203 with 100% probability.

Identifying and diagnosing distinct medication-disease interactions is the main obstacle in drug repurposing. Several AI methods can significantly medication use and repurposing during the COVID-19 pandemic. Mohanty et al. employed machine

learning, deep learning, RNNs, CNNs, and deep belief network algorithms to quickly and precisely screen and output the needed medications after using the Repurpose Drug Database and Open Chemical/Drug Database as inputs for their model.

With the use of this method, pharmaceuticals can be repurposed without first undergoing toxicity testing, enabling the direct use of changed drugs in late-stage treatment. A key component of COVID-19 drug development is phenotype-based compound screening, which employs gene expression patterns and has advantages over target-based drug discovery. Researchers have used a mechanism-driven neural network technique known as DeepCE, which combines graph neural networks with mechanisms for multi-head attention. This method predicts distinct gene expression profiles impacted by unique chemical entities by modelling the connections between chemical substructures and genes as well as gene–gene interactions. To improve the data, the researchers also pulled useful information from the L1000 dataset. This technique was used to repurpose medications for COVID-19. Ten new lead chemicals, including cyclosporine and chloramphenicol, that are consistent with the clinical findings were successfully identified by the researchers. [51]

LIST OF AI TOOLS EMPLOYED IN DRUG DISCOVERY

1) NEURAL GRAPH FINGERPRINTS:

It is employed to forecast the new molecule. You can use it by going to https://github.com/HIPS/neural-fingerprint. For the majority of medications to be found using virtual screening, they must be encoded as a fixed-size vector called a molecular fingerprint. One well-liked molecular fingerprint is the extended connectivity fingerprint (ECFP). In terms of interpretability, parsimony, and predictive performance, these neural graph fingerprints perform better than fixed fingerprints.

2) DeepTOX:

It is employed to forecast toxicity. You can use it by going to www.bioinf.jku.at/research/DeepTox. Deep Learning inherently facilitates multi-task learning, which involves learning all harmful effects in a single neural network, hence learning highly informative chemical characteristics. The DeepTox pipeline was developed to predict toxicity using deep learning. The first step of DeepTox is to normalise the substances' chemical representations. After that, a lot of chemical descriptors are calculated and fed into machine learning techniques. After that, DeepTox trains models, assesses them, and creates ensembles by combining the best of them. At last, DeepTox forecasts the toxicity of novel substances.

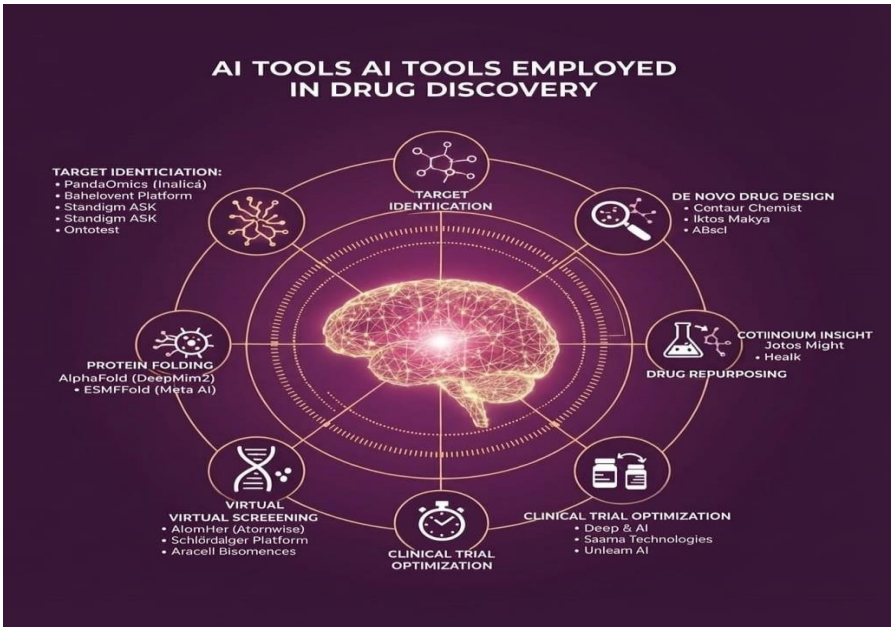

Figure 5: AI Tools Employed In Drug Discovery

3)DeepNeuralNet QSAR:

It is employed in the prediction of molecular activity. You can use it by going to https://github.com/Merck/DeepNeuralNet-QSAR.

Quantitative structure-activity relationship (QSAR) models are often employed computational techniques in the drug discovery process. QSAR models are regression or classification models that use molecular structural features to forecast a molecule's biological activity. (fig:6)These models are usually used to help scientists better understand how structural changes impact a molecule's biological functions and to prioritise a list of potential molecules for upcoming lab trials.

4) ORGANIC:

This effective molecular production tool produces compounds with desired characteristics.

You can use it by going to https://github. com/aspuru-guzik-group/ORGANIC. Based on Objective-Reinforced Generative Adversarial Networks (ORGAN), ORGANIC is a framework that can produce a distribution over molecular space that satisfies a set of desired metrics. This approach combines two machine learning techniques: Reinforcement Learning (RL) to bias this generative distribution towards particular qualities and a Generative Adversarial Network (GAN) to produce non-repetitive sensible molecular species.

5) DEEPCHEM:

It is employed in a number of drug discovery job forecasts. To use it, go to https://github.com/deepchem/deepchem.

DeepChem is developed in Python and offers a feature-rich set of capabilities for using deep learning to solve cheminformatics and drug discovery issues. Chemiformatics has used earlier deep learning frameworks, such as scikitlearn, but DeepChem is the first to use NVIDIA GPUs to speed up computation.[52]

APPLICATION OF AI IN THE PHARMACEUTICAL INDUSTRY

From excipient selection and synthesis pathway prediction to process optimisation, drug design, supply chain, and preventative maintenance, among other areas, artificial intelligence is radically changing the pharmaceutical production process. AI's application in medicine Businesses have the ability to save a substantial amount of money and time at different phases of medication research and discovery. By identifying chemicals more rapidly and precisely predicting their effects, AI speeds up hit identification, lead optimisation, and preclinical testing. The drug discovery process, which typically takes three to six years, can be expedited by AI-driven technologies. AI can shorten this period by one to two years by more accurately predicting therapeutic efficacy, toxicity, and ideal molecular configurations.

The average cost of producing a new drug is approximately $2.8 billion, of which 35% can be attributed to the cost of drug discovery [53]. AI can lower the cost of drug discovery by testing fewer molecules and enhancing the early-phase trial success rates. AI can also help optimise clinical trial designs, including patient recruitment, patient monitoring, and cutting trial duration and cost. By automating data gathering and processing, AI can help shorten the time required for clinical trials, enabling more effective patient outcome monitoring. Trials have been shortened by 15 to 30 percent as a result [54].

AI can help shorten the time it takes for medications to transition from Phase I to Phase III by anticipating side effects earlier and improving dosage techniques. AI-identified molecules have shown greater success rates in early stage clinical studies in contrast to those found by conventional techniques. Compared to the previous industry standards of 40–65%, phase 1 trials for AI-discovered medications have attained success rates of 80–90%. The success rate for AI-discovered compounds in Phase 2 trials is about 40%, which is similar to past averages. The pharmaceutical industry may witness an increase in the likelihood of a drug successfully completing all clinical phases from 5–10% to 9-18% if these trends persist into phase 3 and beyond.(55)

AI BASED ADVANCED APPLICATIONS

AI BASED NANOROBOTICS FOR DRUG DELIVERY

The primary components of nanorobots are integrated circuits, sensors, power supplies, and safe data backups that are maintained by computational technologies like artificial intelligence [56]. They are designed to prevent the collision, identify the target, find and attach it, and then expel it from the body. The capacity of advanced nano/microrobots to navigate to the targeted region based on physiological parameters, such pH, improves their efficacy and lowers systemic adverse effects [57]. When developing implantable nanorobots for controlled drug and gene delivery, factors like dose adjustment, sustained release, and control release must be taken into account. Additionally, the drugs must be released automatically using AI tools like NNs, fuzzy logic, and integrators [58]. Microchip implants are utilised for both programmed release and implant location detection.

AI EMERGENCE IN NANOMEDICINE

For the effective diagnosis, treatment, and surveillance of intricate diseases like HIV, cancer, malaria, asthma, and multiple inflammatory disorders, nanomedicines employ nanotechnology with medications. Due to their improved efficacy and treatment, drug delivery modified by nanoparticles has gained importance in recent years , within the domains of therapeutic and diagnostics [59]. Many formulation development issues could be resolved by combining nanotechnology and artificial intelligence [60]. By examining the energy produced during the drug molecules' contact and keeping an eye on the circumstances that can cause the formulation to aggregate, a methotrexate nanosuspension was computationally created .

Chemical calculations and coarse-grained modelling can help determine drug-dendrimer interactions and assess drug encapsulation with within the dendrimer. In addition , the impact of surface chemistry properties on the internalisation of nanoparticles into cells can be investigated using programs like LAMMPS and GROMACS [61].

CURRENT CHALLENGES AND LIMITATIONS

DATA QUALITY AND AVAILABILITY

The availability of high quality annotated datasets for model training is a major obstacle in AIpowered drug development. A major obstacle is data heterogeneity, which occurs when data originate from many sources including chemical structures, biological assays, and clinical trials. Combining and coordinating these various data sources into a single AI training formats can be intricate and time-consuming [62]. Additionally, biases in the training data might have a significant influence on the robustness, dependability along with model performance ; For instance, the resulting model may show biases that restrict its generalisability and accuracy in practical applications if a dataset mostly represents a particular demographic or disease subset [63,64]. Careful data curation, reliable data pretreatment procedures, along with the development of strategies to migrate bias and guarantee data representativeness are all necessary in order to address these limitations.

INTERPRETABILITY AND TRANSPARENCY

The intrinsic complexity and opacity of AI systems provide a serious obstacle to their mainstream adoption. Many AI models, most notably DNNs, operate as "black boxes," making it difficult to understand the logic underlying their choices [65]. Concerns around trust, accountability, and the potential for inadvertent bias. In the healthcare industry, for example, it is essential for doctors to comprehend the logic behind an AI-powered diagnostic systems aimed at enabling to make well-informed judgements and guarantee patient safety [66].

INTEGRATION IN TO EXISTING DRUG DEVELOPMENT PROCESS

There are many obstacles to overcome when integrating AI techniques into current drug development processes. Rigid protocols and a heavy focus on established methodologies are common characteristics of traditional pharmaceutical operations [67]. The current infrastructure, workflows, and skills may need to be substantially modified to incorporate AI technologies . Adoption of these technologies may also be hampered by worries about data privacy, intellectual property, and the possible effects of AI on jobs in the pharmaceutical sector. [68]

FUTURE PROSPECTIVES

It is anticipated that AI-driven methods will become more and more prevalent in the future of drug discovery, allowing for improved comprehension of disease physiopathology and more precise predictions of drug-target interactions. AI models are going to trained using larger biological datasets, including as proteomics, metabolomics, genomes, and patient data from clinical trials, to find new drug candidates and optimise drug design to lower the chance of clinical trial failure [69-71].

Furthermore, AI has the potential to revolutionize the design and execution of clinical trials in general by enhancing patient recruitment, monitoring, and data analysis. This is because sophisticated algorithms will make it possible to identify qualified candidates based on genetic and phenotypic profiles, guaranteeing that trials are carried out with the most suitable cohort of participants [72-74]

By using Big Data to customise treatments for each patient, AI will keep accelerating the development of personalised medications. Because genetic, environmental, and lifestyle data can be analysed, highly customised treatment approaches will continue to be widely used, taking into account each patient's unique demands [75,76]. While predictive maintenance algorithms will minimise downtime and prevent equipment breakdowns, AI-driven digital twins will simulate and optimise manufacturing processes in real-time, enabling more responsive and agile manufacturing operations [77].

For example, the Health Insurance Portability and Accountability Act (HIPAA) Privacy Rule in the United States sets national standards to protect

individuals' medical records and other identifiable health information, commonly referred to as protected health information (PHI). This regulation applies to healthcare providers, health plans, and healthcare clearinghouses that engage in specific electronic healthcare transactions [78].

DISCUSSION:

Owing to its capacity to deliver rapid , data-driven insights that conventional approaches are unable to provide, artificial intelligence has emerged as a potent force in contemporary drug discovery. Large biological and chemical datasets are analysed by AI techniques to rank compounds early in the discovery process, predict interactions, and uncover disease-related targets. When compared to traditional trial-and-error methods, this greatly reduces delays and increases accuracy. Deep learning scoring systems, generative models, and AI-based virtual screening have improved lead optimisation and hit detection. These methods provide new chemical compounds with enhanced drug-like characteristics while enabling effective prediction of binding affinity, molecular properties, and toxicity. Consequently , AI minimizes the need for labor – intensive experimental screening efforts thus creating new opportunities of early identification of good candidates. AI aids in pharmacokinetic modelling, toxicity evaluation, and ADMET prediction in preclinical and clinical research, assisting in the removal of inappropriate compounds prior to costly testing. Through improved patient selection, adaptive trial designs, and digital twin simulations, AI also enhances clinical trials, ultimately lowering failure rates and raising trial efficiency. Nevertheless, there are still obstacles in the way of completely incorporating AI into pharmaceutical processes. Regulatory acceptance, model transparency, and data quality remain significant challenges. Many sophisticated models function as "black boxes," which restricts trust and interpretability. Strong computing infrastructure, knowledgeable staff, and explicit policies about data privacy and intellectual property are also necessary for incorporating AI. For AI-driven drug discovery to be widely used, these problems must be resolved.

CONCLUSION:

With its creative answers to many of the shortcomings of conventional research approaches, artificial intelligence has emerged as a crucial pillar in current drug development. AI significantly reduces the time, cost, and uncertainty associated with drug development by enabling rapid target identification, more precise molecular behaviour prediction, and effective lead compound optimisation. Its use goes beyond early discovery; it has an impact on formulation design, clinical trial optimisation, preclinical modelling, toxicity prediction, and personalised medicine. Neural networks, generative models, and digital twins are examples of AI-driven tools that significantly improve decision-making and success rates along the pharmaceutical pipeline. Despite these advancements ,challenges related to data quality, model interpretability, ethical use, and regulatory compliance, current technology developments and trends in worldwide acceptance show that AI will continue to transform the pharmaceutical industry. As integration grows, AI offers safer clinical trials, more precise treatments, fewer development failures, and quicker access to new medications—all of which will improve patient outcomes and influence the direction of global healthcare in the future.

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