ARTIFICIAL INTELLIGENCE IN DRUG DISCOVERY AND DEVELOPMENT: AN OVERVIEW OF EMERGING ROLES AND TECHNIQUES

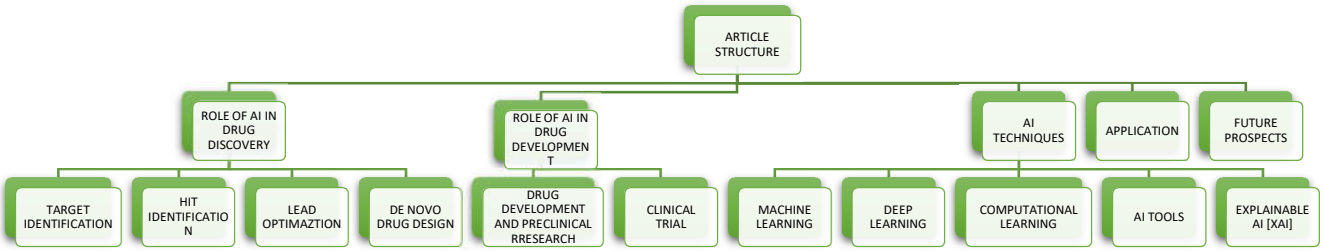
Dr. Senthil Rajan. D*, Mr. Devanandh. D*, Ms. Kaveena Ravi*, Logeshwari. D, Sivareshma. S, Sriharini. G, Subalakshmi. M, Varsha. T

Department of Pharmaceutics, Swamy Vivekanandha College of Pharmacy,

Tiruchengode, Namakkal(DT), Tamilnadu, India - 637205.

Affiliated to the The Tamilnadu Dr. M.G.R. Medical University, Guindy, Chennai – 600032.

ARTICLE BACKGROUND:



ABSTRACT:

Artificial intelligence with its unparalleled speed, accuracy, and predictive power throughout the pharmaceutical research pipeline. Artificial intelligence (AI) has become a revolutionary force in contemporary drug discovery and development through sophisticated computational models. Artificial intelligence facilitates creative de novo drug design, expedites target identification, improves hit identification, and supports effective lead optimization in early discovery. AI driven tools in drug development facilitate pharmacokinetic and pharmacodynamic profile in the field of prediction, enhance decision making, and optimize formulation strategies. Additionally, AI greatly improves clinical trial design, patient recruitment, monitoring, and outcome prediction, while cutting costs and time. Building transparent, comprehensible, and trustworthy models for pharmaceutical applications is facilitated by fundamental AI techniques like machine learning, deep learning, computational learning, and explainable AI. This article offers a through summary of the various applications of AI in drug development and discovery, highlighting its potential to transform therapeutic innovation and expedite the molecule-to-market process.

KEYWORDS:

Artificial intelligence, Drug discovery, Drug development, Clinical trials.

1. INTRODUCTION:

AI is a branch of computer science that seeks to understand how that the brain of humans makes choices and solves challenges. The process of finding and developing new drugs is complicated, expensive, and time-consuming. The application of AI and ML in drug development has already shown encouraging results in a number of areas, including lead optimization, virtual screening [1], chemical creation [2], medication repurposing [3] and extensive clinical evaluation. AI speeds up target identification, finds promising hits from large chemical libraries, improves lead optimization through predictive modelling, and supports the de novo design of entirely new molecules with desired biological properties during the drug discovery phase. Target identification, hit identification, absorption, distribution, metabolism, elimination, toxicity prediction, lead optimisation, and drug repositioning are just a few of the stages of drug research where artificial intelligence is used [5]. AI helps with formulation research in ADMET evaluation and process optimization at the drug development level, which results in shorter development cycles and lower failure rates. By enhancing patient selection, trial monitoring, adherence prediction, and data analysis. AI also significantly contributes to clinical trials, ultimately boosting trial efficiency and reliability. The capabilities of AI in the pharmaceutical industry have been further extended by developments in machine learning, deep learning, computational learning, and explainable AI (XAI). The goal of XAI is to logically explain an AI system's behaviour and decision-making to a users [4]. These methods make AI-driven systems more transparent and reliable by facilitating automation, pattern recognition, and interpretability. It is possible to achieve unsupervised machine learning (ML) outputs like disease target discovery from detection of features techniques and disease category research from clustering [6]. The pharmaceutical industry has turned to artificial intelligence (AI) as a potent enabler that can speed up research workflows and improve decision accuracy in response to growing demands for safe, effective, and customized therapies.AI offers data-driven insights that help researchers create new compounds, anticipate drug-target interactions, comprehend disease mechanisms, and enhance developmental outcomes.

2. ROLE OF DRUG DISOVERY

2.1. TARGET IDENTIFICATION:

Target identification is the very initial stage of drug research, in which researchers strive to identify molecules in the body whose modification by small compounds might result in medical benefits. The conventional methods depend on systematic reviews, genetic investigations, and phenotypic screening, which can frequently take decades of research[7].AI has aided this process by allowing for systematic assessment of multi-omics datasets, including as genomes, transcriptomics, as well as metabolomics data, in order to discover targets responsive to minor-molecule intervention[8].Nearest- Neighbour classifiers, extreme learning machines, supervised learning (SVMs), and deep neural networks (DNNs) are employed for virtual screening based on synthesizing effectiveness, and they are capable of predicting in vivo activity and toxicity [9,10].

2.1.1. MULTI OMICS DATA SET:

A substantial quantity of data can be added to multi-omics data sets using a variety of omics technologies. They are proteomics, metabolomics & genomics. With the help of AI and data processing methods, researchers can manage and examine these enormous, varied data sets. One of AI's main benefits in multi-omics research is the automation and simplification of data processing and analysis operations [11].

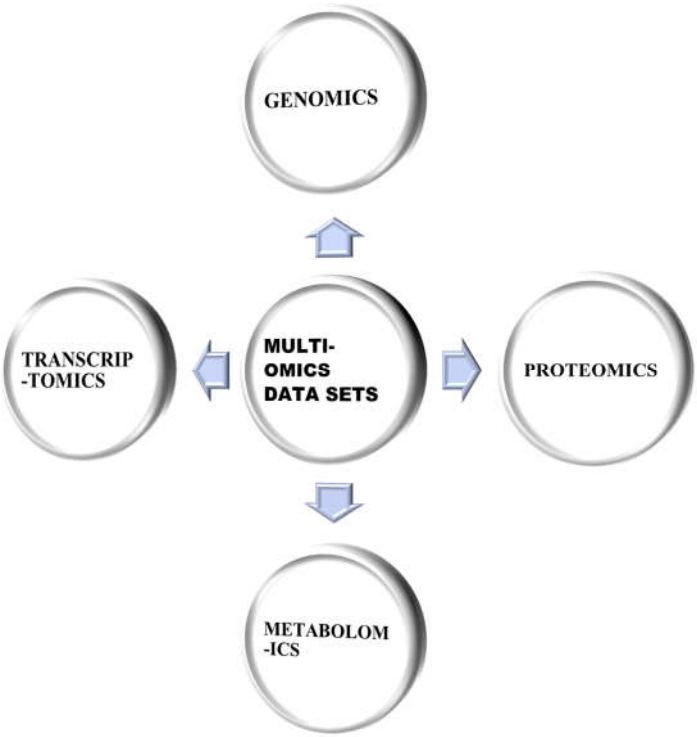


Fig 1: MULTIOMICS DATA SETS

- **GENOMICS:**

Understanding the entire genetic makeup of an organism, which includes all of its genes and non-coding sections is crucial. This type of information includes identifying genetic variations and figuring out how they connect to particular characteristics and diseases, as well as examining the sequencing, structure, and function of DNA. Two of the primary technologies utilized in genomics are genotyping and DNA sequencing DNA sequencing includes ascertaining the nucleotide order in a DNA molecule, whereas genotyping involves identifying genetic differences, such as single nucleotide polymorphisms (SNPs), in a specific region of the genome [12].

Finding mutations that cause disease, predicting treatment outcomes, and population genetics studies are all uses for genomic data. For example, genomic data has been used to identify cancer cell mutations that stimulate tumor growth and to develop targeted therapies that target these mutations directly [13].

- **PROTEOMICS:**

Proteomics is the study of every protein that a cell, tissue, or organism expresses. This important kind of multi-omics data can provide insight into the functional and regulatory networks that govern cellular functions. Proteomics data can be generated using a variety of techniques, including high-throughput sequencing, mass spectrometry, and protein microarrays [14-16]. One of the main applications of proteomics is the discovery of biomarkers for illness diagnosis and prognosis.

- **METABOLOMICS:**

Metabolomics is the study of metabolic products, or tiny compounds, present in biological fluids, tissues, and cells. Metabolites which are products of biological processes can provide insights into how cells function as well as the effects of external factors like diet, exercise, and environmental exposure. Metabolites are frequently detected and measured in metabolomics processes using mass spectrometry, nuclear magnetic resonance, or other analytical methods [17].

2.2. HIT IDENTIFICATION AND VIRTUAL SCREENNG:

Primary "hit" compounds in a biochemical experiment are identified by a positive response during the initial screening phase. Further screening is then carried out to determine whether the hit compounds' pharmacological and physicochemical characteristics are appropriate for creating a medication. They are classified as "leads" if they make it through this filter. Before moving on to clinical testing, these leads are first chemically improved and then put through biological assessment in later rounds. It may take 12 to 15 years from the start of testing for a lead to eventually be approved as a medication [18].

Repositioning drugs for uncommon illnesses We provide an example of drug repositioning for uncommon disorders in this section. The most prevalent inflammatory muscle illness among older persons is IBM (inclusion body myositis), which is regarded as an uncommon condition with a relatively low prevalence rate. Progressive muscle weakening that gradually results in severe impairment is its defining feature. In this instance, we have simulated a microarray dataset from muscle tissue biopsy.[19]

2.3. LEAD OPTIMIZATION IN AI:

AI has improved lead optimization by employing multi-objective optimization algorithms, which are more effective than conventional approaches at navigating intricate property environments. When considering small-molecule optimization as a sequential decision-making problem, where chemical alterations are chosen to optimize a reward function that encodes the desired attributes reinforcement learning techniques have demonstrated promise [20,21].

These methods can simultaneously maximize several goals while preserving synthetic accessibility and chemical validity. However, as criticized in [22]reinforcement programming can be sample-inefficient and vulnerable to local optima. It lessens adverse effects and increases medication effectiveness. It lowers the expense and time of discovery.

2.4. DE NOVO DRUG DESIGN IN DRUG DISCOVERY:

The goal of drug design is to produce chemical species that satisfy certain requirements, such as sufficient innovation to guarantee intellectual property rights for commercial success a reasonable safety profile appropriate chemical, biological features and efficacy against pharmacological target or targets.

Whether directly adapted from protein structures or deduced from the characteristics of known ligands, early de novo drug design approaches [23]. Nearly solely employed structure-based techniques to build ligands within the constraints (steric and electronic) of a binding pocket for the target of interest [24,25].

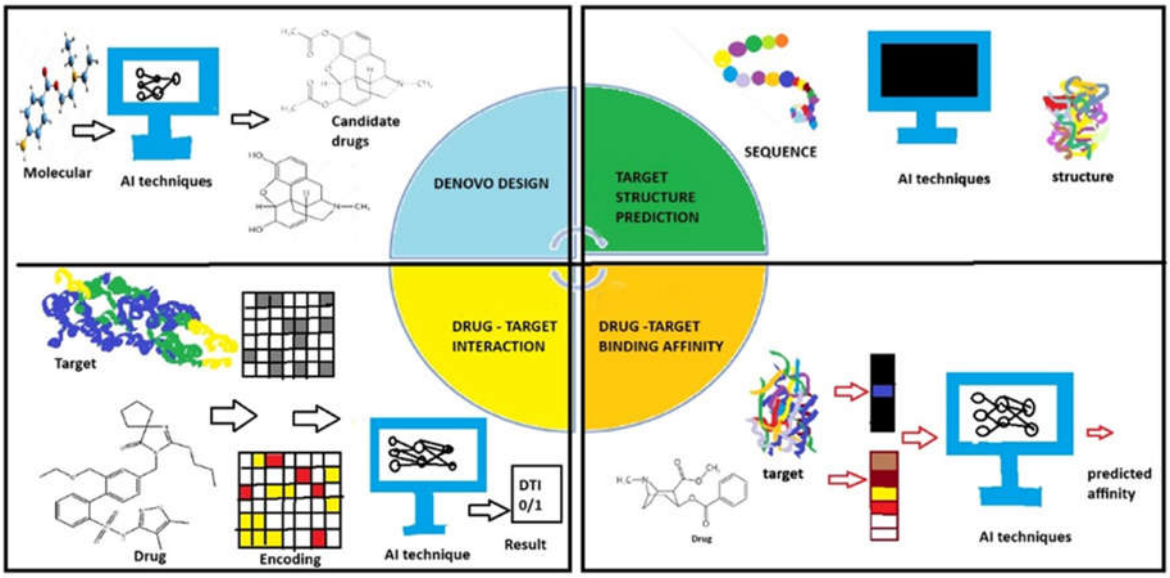


Fig 2: ROLE OF AI IN DRUG DISCOVERY

3. ROLE OF AI IN DRUG DEVELOPMENT

3.1. AI IN DRIVEN DRUG DEVELOPMENT:

Over the past decade, AI technology has transformed pharmaceutical research ushering in a new age of medication development as well as medicine discovery, testing, and patient delivery. This technological advancement has the potential to change the drug development pipeline at multiple phases from expediting preclinical research to enhancing clinical trial design and allowing personalized medicine methods.

- **Boosting preclinical research:**

Preclinical research entails and time-consuming safety and effectiveness evaluations of prospective therapeutic candidates. This method is costly, difficult, and frequently ineffective. AI can improve data processing, anticipate medication interactions, and uncover potential molecules. Machine learning algorithms have been created to estimate the toxicity of possible medication candidates [26]. Using AI-powered systems the researchers may swiftly screen hundreds of medications and pick the most appealing possibilities, greatly lowering the duration and expense of preclinical testing [27].

3.2. Clinical trial design optimization:

Conventional trial designs are frequently defective and inefficient, resulting in high expenditures, extended timetables, and occasionally ambiguous outcomes. By using predictive analytics to adapt inclusion criteria and treatment procedures, AI can enhance patient enrolment , trial results, and innovative medicine development [28]. AI algorithms can assess patient data, discover biomarkers, and stratify groups to enhance trial design [29]. Before launching costly and time-consuming clinical trials the researchers may use AI-powered simulations to explore virtual trial situations, optimize study procedures, and limit risks.

✓ **Personalised medicine methods:**

One of the most potential uses of Artificial intelligence in drug research is accelerating the development of customized medicine. The illness treatment and medication development framework is evolving toward customized medicines in order to get superior outcomes for specific individuals. AI has the potential to accelerate this trend by enhancing diagnoses, gathering tailored data, and aiding with healthcare decisions [30]. AI algorithms may store and evaluate patient data including genetic profiles, clinical histories, and lifestyle factors [31]. This can greatly reduce the load of comprehensive data gathering and analysis on researchers allowing them to focus on the clinical case and complete their work quickly and efficiently.

Furthermore, AI technology can detect biomarkers related with treatment responses or disease progression, hence enhancing tailored therapies with maximum efficacy and lowest side effects[32]. Finally, AI-driven drug development has the potential to revolutionize the pharmaceutical sector by improving preclinical research, clinical trial design, and individualized therapy. AI can help researchers find and deliver novel treatments that meet clinical needs and enhance patient outcomes.

✓ **The path to clinical trials for drug safety:**

Prior to first-in-human studies, preclinical safety evaluation includes both in vitro and in vivo testing to assure patient safety. In vitro toxicology testing is intended to detect toxicities that may have a serious impact on the progression in a drug discovery process. It is available in a variety of assay formats, ranging from standard single-end point screening to more. Lately, complicated in vitro model systems, such as micro physiology or organ-on-chip models. These are used before or alongside in vivo experiments. AI advancements in this area include the integration of varied, more sophisticated data types (e.g., gene expression, cell painting), along with a larger use of imaging for a range of tasks related to data processing.

✓ **Predictive toxicology:**

A tiny-molecule MPO design (discussed above) involves estimating in vitro organs toxicity such as cytotoxic and mitochondrial toxicity, being part as appropriate diagnostics for determining outside-target toxicities and DNA toxicity (33). Further advances incorporate analysing emerging data formats such as gene transcription data and cell imaging data in conjunction with chemical structure information to estimate in vivo toxicity-associated impacts (34). Pharmacological DNA fingerprints, either independently or in conjunction with anatomical DNA fingerprints, can better tie chemicals to in vivo phenotypes, perhaps with

more predictability (35).Modelling has been more prevalent in clinical drug development during the last decade, as shown by a rise in legislative publications (ICH, 1997) and pharmaceutical firm reports(36-38) and conference reports/position papers (39,40). Several investigations have demonstrated that the strategy is cost-effective (41). The majority of these attempts have focused towards the investigation of data from clinical trials. Despite pharmacokinetic and psychometric modelling proved to be employed in phase I for a longer duration than in subsequent phases, they do not appear to possess been a significant influence upon clinical drug development (42).

Drug discovery is the process of developing medications that eliminated or treat illness. As stated by the writers in [43], the typical length of investigation and development for the production of an entirely novel form of medication is between ten and seventeen decades, including a projected median price tag of well over United States $ 2.8 billion each year. Further hurdles exist with these studies, particularly the poor efficacy and high expense of traditional approaches for drug discovery [44]. A Detailed Investigation, as a result there's an obligation to create innovative strategies to mitigate these issues.

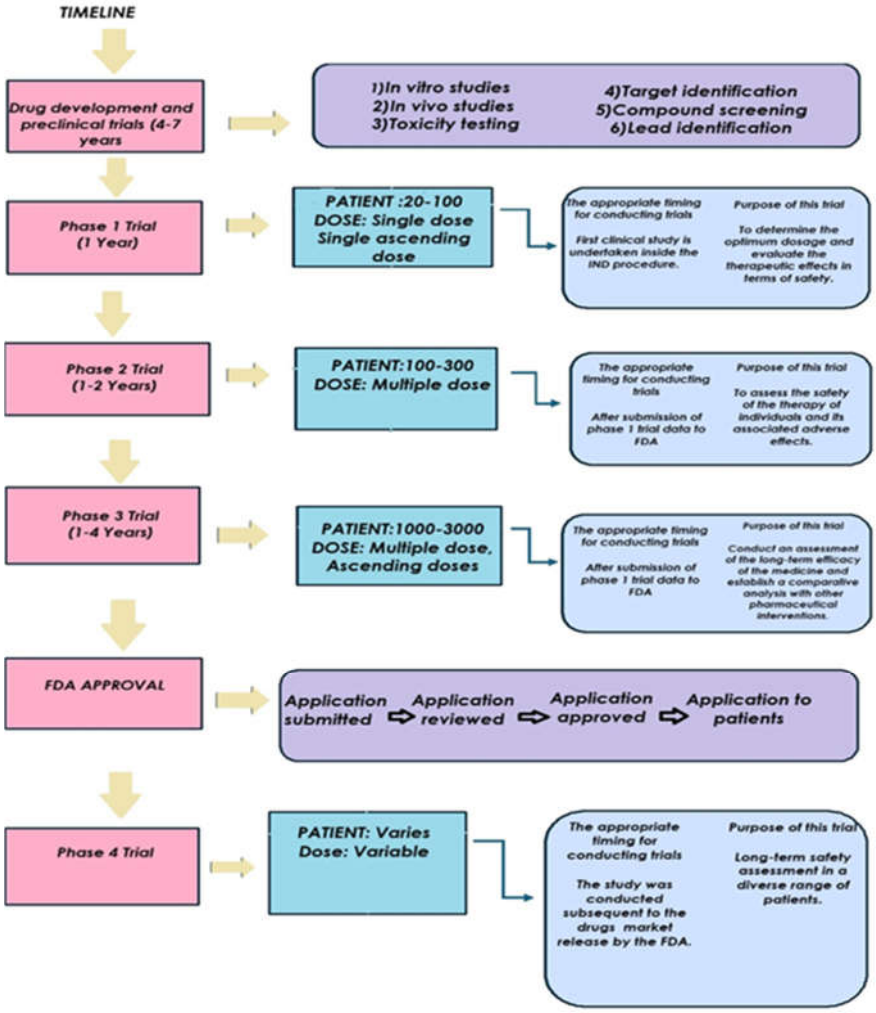


Fig 3: ROLE OF AI IN DRUG DEVELOPMENT

4. AI TECHNIQUES:

4.1. MACHINE LEARNING:

AI is defined as the use of techniques that allow machines to simulate human behaviour. AI additionally involves a topic termed Machine learning (ML), that employs methods from statistics to learn in conjunction with or without explicitly coding [45-47].

Machine learning is divided into three main groups:

- Unsupervised,
- Supervised,
- Reinforcement learning.

Many of numerous ways that machine learning can help researchers reduce errors include: Analysing patient demographic information to identify the traits of persons that are most likely to gain advantages from the suggested therapy or modification (often described generically as "responding patients") hence enhancing trial selection of groups improving the procedures of locating as well as enrolling participants in studies such example, by leveraging HER data to link patients with trials. [48,49].

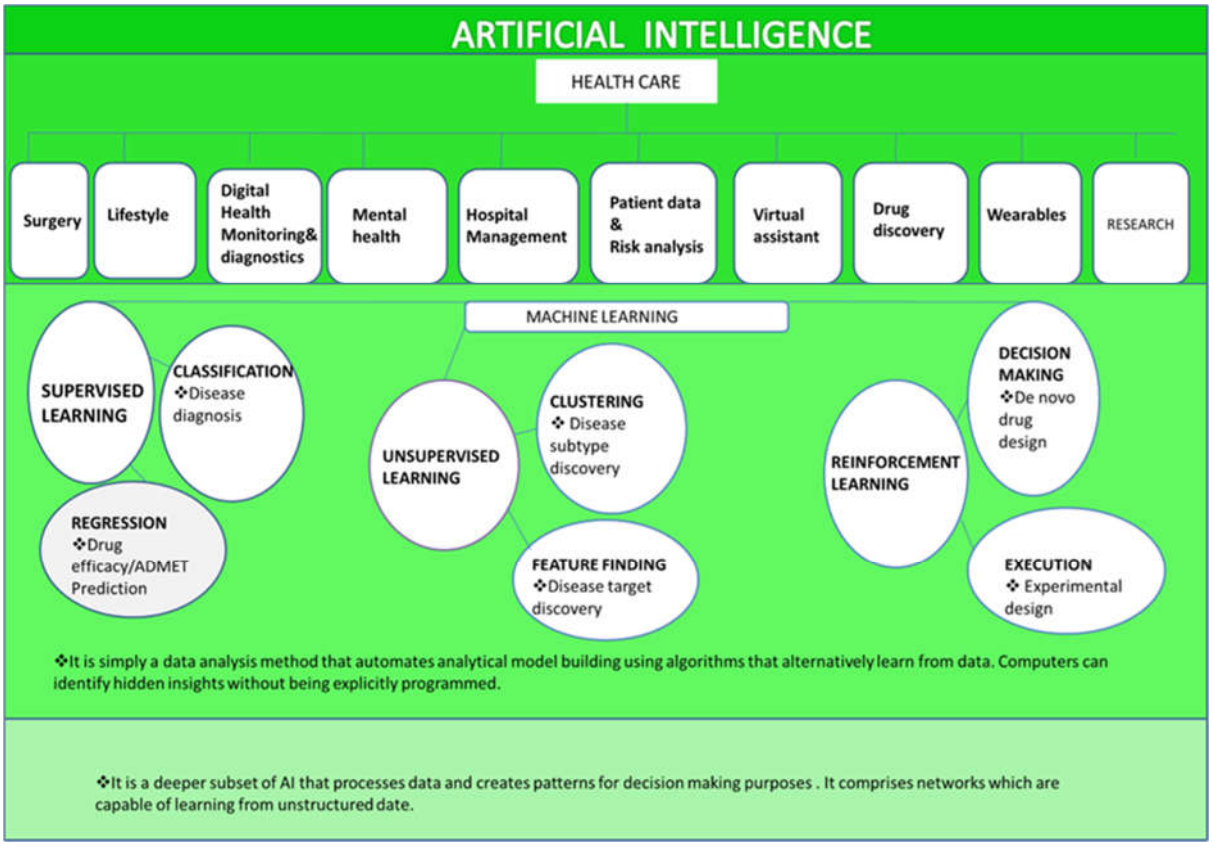


Fig 4: AI IN MACHINE LEARNING

4.1.1. SUPERVISIED LEARNING:

- **Prediction of Absorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) using AI guidance:**

AI approaches can accurately anticipate medication absorption, distribution, metabolism, excretion and toxicity features. Predictive models use designed and learnt molecular characteristics to anticipate human intestinal absorption (HIA). Caco-2 cell permeability and parallel artificial membrane permeability are examples of in vitro experiments that indicate absorbing ability. Extensive information allow for the creation of prediction models for drug-protein binding, P-gp restriction and Blood Brain Barrier (BBB) permeability. Accurate estimates for Blood Brain Barrier permeability, cytochrome P450 (CYP) enzyme substrate and inhibitor interactions, plasma half- lives, solubility, metabolic stability, potential metabolites, renal excretion, bile salt export pump (BSEP) inhibition, hepatotoxicity assessment and cardiac toxicity can be made by investigating machine learning (ML) models, molecular descriptors and structure-activity relationships [50-61].

- **Drug Repurposing:**

The challenge in computerized drug reuse stems from the scarcity of known links connecting domains (medicine, destination and illness) in addition to the vast number of hypothetical relationships that must be forecasted. The total number of recognized correlations from accessible databases remains fairly minimal in comparison to the overall pharmacological field.

The method of Laplacian structured least-squares [62,63], a well-known supervised learning technique for drug repurposing was used to forecast pharmacological-target relationships with prospective uses of authorized by the Food and Drug Administration (FDA) pharmaceuticals found through target prediction. LapRLS creates two distinct environments for medicines and targets.

4.1.2. UNSUPERVISED LEARNING:

- **CLUSTERING:**

Although machine learning (ML) may be used for categorization or clustering patients based on several factors at the same time, there is yet no data or instances to show that AI outperforms traditional statistical approaches in clinical care. Biomarker-powered adaptive trials, which include the BATTLE-2 trial [64] may be divided into three phases: training, testing, and validation, a process comparable to machine learning procedures. As a result, developments in AI, such as deep learning, may prove advantageous when used to adaptive trials.

4.1.3. REINFORCEMENT LEARNING:

- **DE NOVO DRUG DESIGN:**

De novo design, the creation of unique molecular components with expected therapeutic properties from beginning to end [65], is one of the most complex computationally supported drug discovery assignments due to the dual nature of the chemical domain of molecules that resemble drugs (which is estimated to be on the order of 1060-10100) [66,67].

Ligand-based strategies can be separated into two major categories: (i) rule-based approaches, that make use of a variety of creation rules for structure assembly using a set of 'building blocks' (i.e. reagents or molecular fragments) and (ii) rule-free approaches, which have no specific synthesis rules.

Synthesis-oriented techniques clearly provide instructions for assembling building blocks and producing ligands. These methods are important in designing synthetically accessible libraries [68,69], such as BI CLAIM [70] and CHIPMUNK [71]. Throughout the later 1990s, hybrid techniques like as TOPAS [72], DOGS [73], and DINGOS [74] were been established to direct the synthesis of new molecules by optimizing each their resemblance to known bioactive ligands and the chemical synthesis capability of the designs. 'Rule-free' techniques try to build molecules with specified characteristics without the use of chemical construction rules.

Recent techniques frequently use dynamic deep learning models [75] to isolate novel compounds from a previously acquired underlying chemical information. While these techniques have grown in popularity in recent years, the concept of sampling from a numerical illustration of chemicals for de novo design traces back to the beginning of the 1990s, when Skvortsova and Zefirov proposed the 'inverse QSAR' problem. Inverted QSAR employs a previously developed QSAR model to find the descriptor values correlating to a desired attribute and then uses this knowledge for molecule creation [76-79].

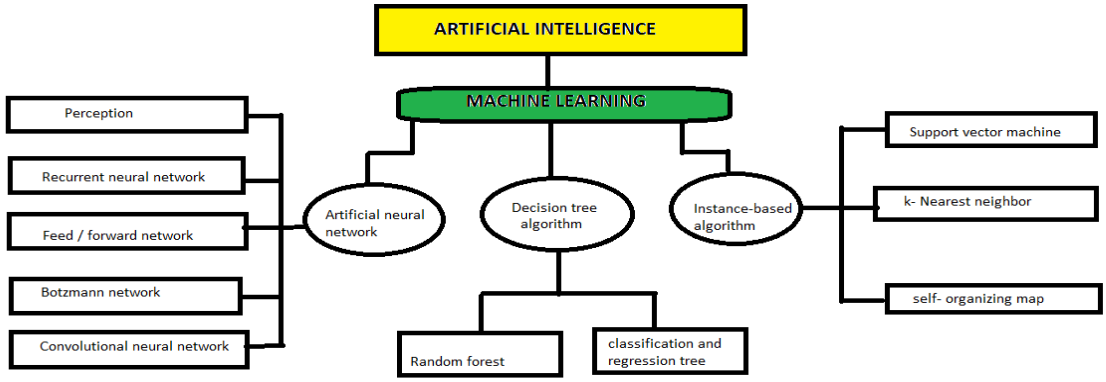


Fig 5: AI IN MACHINE LEARNING NETWORK

4.2. Deep learning:

In order to replicate the functioning of the human central nervous system (CNS), deep learning is a redesign of a conventional machine learning (ML) method known as artificial neural network (ANN), which is a network system made up of interconnected artificial neurons (80).

Predicting drug-target interactions (DTIs), creating new compounds and estimating absorption, distribution, metabolism, excretion and toxicity (ADMET) features for translational studies are three of the primary fields in computational chemistry where Deep Learning models have been documented (81). Deep Learning is increasingly being used to create QSAR/QSPR models, much as other Machine Learning techniques. Hilton's team used their Deep Learning models to win the Merck Kaggle challenge (https://www.kaggle.com/c/MerckActivity) as far back as 2012, initiating an entirely fresh chapter in the use of Deep Learning techniques for predicting the activity patterns and properties of chemical compounds. In an identical manner, Wang and Zeng used Restricted Boltzmann Machine (RBM), the widely acknowledged initial release of Deep neural networks (DNN) to publish their DTI discriminatory model (82).

4.2.1. Networks of deep learning:

Artificial neural networks with several hidden layers are used in deep learning, a particular form of machine learning, to automatically extract high-level characteristics from unprocessed data. Thammana PK and Sarella PN. Folate-conjugated chitosan nanoparticles have potential uses in the targeted administration of anticancer medications.

Deep learning can be very helpful in drug stability studies when managing big, unstructured datasets and modelling intricate non-linear interactions.

Predictive analytics frequently makes use of the following deep learning architectures:

- **CNN or convolutional neural networks:** CNNs are excellent for interpreting spectroscopic or chromatographic data that may be pertinent to drug stability investigations since they excel at image and signal processing tasks.
- **Recurrent Neural Networks (RNNs):** RNNs may be utilized for modelling data with time series, such as atmospheric data collected from sensors or 24-hour stability monitoring, because they are made to handle data in sequence.
- **Long Short-Term Memory (LSTM):** An Recurrent Neural Network version that can efficiently capture dependency relationships over time in sequential data, thus rendering it appropriate for long-term drug stability modelling.
- **Autoencoders:** Unsupervised deep learning models that are capable of learning effective data encodings and representations, which may be helpful for decreasing dimensionality and recognition of features in drug stability data.

- **Generative Adversarial Networks (GAN):** Made up of two rival neural networks (the discriminating network and generators), GANs may be applied to simulate complicated distributions, provide artificial stability data, or enhance data. [83]

Typical Deep Learning Frameworks for Small Molecular Drug Development. Depending on the nature of the training data, various Deep Learning architectures may identify patterns and extract high-level features in different ways. We primarily covered popular designs in this review, such as CNN, RNN and Generative networks (84). An illustration of an AI-based program that can detect skin cancer as accurately as a medical professional. Nearly 130,000 photos of moles, rashes and lesions are recognized by the application using a deep learning approach [85] which aids in the very accurate identification of skin cancer. For fifteen therapeutic candidates absorption, distribution, metabolism, excretion and toxicity (ADMET) data sets, Deep Learning models demonstrated notable predictivity when compared with conventional Machine Learning techniques [86,87].

4.3. COMPUTATIONAL MODELS:

Many drug discovery processes, such as chemical ingredient identification, target recognition, peptide synthesis, drug toxicity, physiochemical property evaluation ,drug monitoring, drug efficacy, effectiveness assessment, bioactive agent prediction, protein-protein interaction, protein folding ,misfolding identification, structure and ligand-based virtual screening (LBVS), QSAR modelling and drug repositioning, have been made possible by computational modelling based on Artificial Intelligence and ML [88].

- **Structure-based modelling using artificial intelligence and QSAR/QSPR:**

QSAR/QSPR analysis has developed significantly since its introduction over 50 years ago [89]. These computational models have an indisputable influence on drug development, as proven by their ability to precisely forecast biological functions and pharmacokinetic features such as absorption, distribution, metabolism, excretion, and toxicity (ADMET) [90-93]. For ligand-based QSAR/QSPR modelling, the structural qualities of molecules (such as pharmacological distribution, physical and chemical characteristics, and chemical classes) are usually transformed into machine-readable values using molecular descriptors [94]. The range of handmade Molecular Descriptors is broad [94], attempting to capture a number of elements of the basic molecular structure. In broadly, QSAR/QSPR strategies have shifted away from less complicated designs like linear regression models and k-nearest neighbours and toward more widely relevant machine learning techniques like the use of support vector machines (SVM) and gradient boosting methods (GBM), with the goal of addressing greater complicated and probably nonlinear connection between the molecular makeup and its physicochemical/biological characteristics, often at this cost of interpretability[95].

4.4. AI TOOLS:

Tools	Reference	Ref. no
DeepChem	https://github.com/deepchem/deepchem	96
DeepTox	www.bioinf.jku.at/research/DeepTox	97
DeepNeuralNetQSAR	https://github.com/Merck/DeepNeuralNet-QSAR	98
ORGANIC	https://github.com/aspuru-guzik-group/ORGANIC	99
PotentialNet	https://pubs.acs.org/doi/full/10.1021/acscentsci.8b00507	100

4.5. EXPLAINABLE AI (XAI):

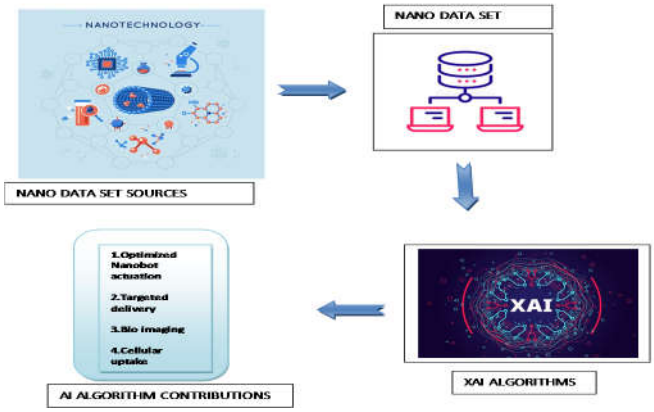


FIG 6: EXPLAINABLE AI

The goal of XAI is to provide a user with a logical explanation of how an AI system behaves and makes decisions [101]. The necessity to explain machine learning model decisions led to the development of XAI in this instance, XAI shows the reasoning a model uses to draw inferences from a classification process. As a result, XAI offers reasoning for system failures, mistake prediction and remedial actions. This permits trust in the model's output [102].

The comparison of well-known XAI models based on the explainability features accuracy and performance metrics is displayed in Robust XAI models are needed for delicate healthcare applications including medication delivery, drug discovery and cancer therapy as we move from weaker to stronger AI.

5. APPLICATION

5.1. AI powered nanorobots for medication delivery:

The primary components of nanorobots are integrated circuits, sensors, power supplies, and safe data backups that are kept up to date by computational technologies like artificial intelligence [103,104]. They are designed to prevent attachment, detection,

collisions and target identification and then be eliminated from the body. The development of nano/microrobots has improved their efficacy and decreased systemic side effects by enabling them to travel to the targeted region depending on physiological parameters [104]. When developing implantable nanorobots for controlled drug and gene delivery, factors like dosage modification, prolonged release, and control release must be taken into account. Additionally, the dispensing from the drugs must be automated and managed by AI tools like Neural Networks (NN), Fuzzy logic, and Integrators [105]. Microchip implants are utilized for both programmed release and implant site detection.

AI in synergism/antagonism prediction and combined medication administration, because they can have a synergistic impact that speeds up recovery, a number of pharmacological combinations are licensed and sold to treat complicated illnesses including cancer and tuberculosis [106,107]. High-throughput screening of a large number of medications is necessary to pick specific and promising pharmaceuticals for combination therapy, which is a laborious procedure. For instance, cancer therapy requires a combination of six or seven drugs. Drug combinations may be screened and the total dosage regimen can be improved using Automated Neural Network (ANN), logistic regression, and network-based modelling [106,108].

5.2. AI use in clinical trials for cardiovascular conditions:

Future research employing AI-guided biomarkers or genomes in advanced adaptive studies may have an influence on every step of the clinical research process, including study design, recruiting, conducting, intervention, and interpreting.[109,110]

5.3. The clinical value of artificial intelligence in cancer therapy:

Constantly evolving, efficient, and novel AI and network healthcare technologies may help to accelerate treatment development (111). Just lately, experts successfully developed a series of ML algorithms to rank therapeutically applicable cancer medications based on their expected efficacy in inhibiting cancer cell proliferation. The findings revealed that machine learning could potentially be extensively used to determine the best cancer therapies for people individually (112).

It is an innovative improvement for the fight against cancer, with the following benefits like the radiation therapy is nonsurgical and painless, it provides beneficial cancer management, and it substantially decreases the possibility of common adverse reactions such as difficulty breathing of breath, trouble with swallowing, or throat inflammation. Therapy are frequently finished in as little as 3 to 5 sessions over a period of one to two weeks, and majority of patients may resume regular routines following treatment like, it is an incredible wonderful technique in cancer therapy.[113]

5.4. AI in combined medication delivery and synergy/antagonistic Prediction:

Multiple combos of medications have been granted approval and commercialized for the management of Chronic illnesses, such as tuberculosis and malignancy with a combined effect for a rapid recovery [114,115]. Researchers effectively predicted 28 synergistic chemotherapeutic combos using this approach, which was built on gene transcription patterns and numerous networks.[116]

5.5. Artificial Intelligence in Drug Repurposing:

The technique of reusing current medications for novel medical treatments is known as "drug repurposing." Drug repurposing provides the benefit of allowing already-approved drugs to avoid phase I clinical trials and toxicity assessment, which lowers development duration as well as hazards [117].

5.6. Predicting Results and Identifying Adverse Effects:

AI can help improve clinical trial safety, safeguard participant health, and detect possible adverse effects early. AI-based result prediction and adverse reaction identification present a chance to improve the effectiveness and dependability of clinical trials, which will be advantageous to both patients as well as investigators.

5.7. Important Problems and Prospects:

Managing the variability across different databases is the main challenge. These databases contain data that was gathered under multiple experimental circumstances and in a different format. Integrated or curated databases have been developed in order to address this issue. [118] To identify the molecular ligand abilities and any safety issues, target drug ability programs has been created, such as Tracta Viewer and Drug Targetor.[119,120]

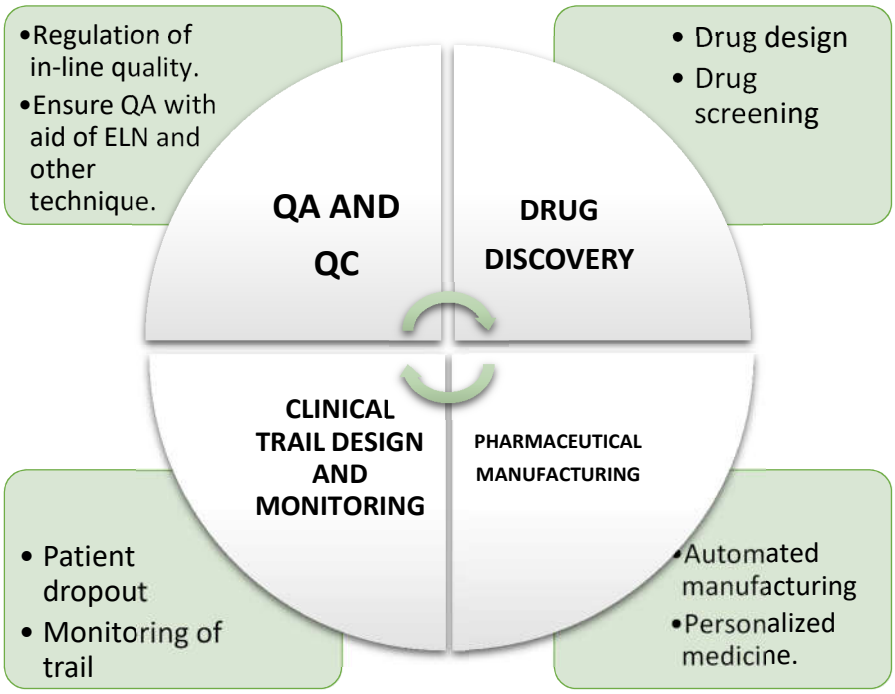


FIG 7: APPLICATION OF AI

CONCLUSION:

Artificial intelligence is emerging as a potent instrument for drug development and discovery. It facilitates the faster and more accurate design of new drugs from scratch, the identification of hit compounds, the optimization of lead molecules, and the discovery of new drug targets. AI helps predict safety, enhance formulations, and increase the effectiveness of clinical trials in drug development. Scientists can analyse complex data and make better

decisions throughout the research process by using techniques like explainable AI, deep learning, and machine learning. In general, AI is accelerating, lowering the cost, and improving the reliability of pharmaceutical research, which will help patients receive better medications sooner.

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113. The Potential Applications of Artificial Intelligence in Drug Discovery and Development Hassan FARGHALI1 , Nikolina KUTINOVÁ CANOVÁ1 , Mahak ARORA1 1 Institute of Pharmacology, First Faculty of Medicine, Charles University and General University Hospital in Prague, Czech Republic Received July 17, 2021 Accepted October 10, 2021.

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