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ARTIFICIAL INTELLIGENCE IN DRUG DEVELOPMENT

Pranshu Patel, Shiv Hardenia * and Dinesh Kumar Jain

IPS Academy College of Pharmacy, Knowledge Village, Rajendra Nagar, A.B. Road, Indore - 452012, Madhya Pradesh, India.

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Correspondence to Author:
Dr. Shiv Hardenia

Associate Professor,
IPS Academy College of Pharmacy, Knowledge Village, Rajendra Nagar, A.B. Road, Indore - 452012, Madhya Pradesh, India.

E-mail: shivsharma280485@gmail.com

ABSTRACT: Artificial intelligence (AI) is rapidly transforming the drug development process, offering innovative solutions to streamline and accelerate the discovery of new therapeutics. Traditionally, drug development has been a time-consuming and costly endeavor, often taking over a decade and billions of dollars to bring a drug to market. AI, with its ability to analyze vast amounts of complex data, has the potential to significantly reduce both time and costs while improving the success rate of new drugs. AI techniques, including machine learning (ML), deep learning (DL), and natural language processing (NLP), are being integrated at various stages of the drug development pipeline. In the early stages, AI is used to analyze large datasets, such as chemical, genomic, and proteomic data, to identify potential therapeutic targets and biomarkers. Machine learning algorithms can also predict a compound's biological activity, optimizing lead compounds and enhancing virtual screening compared to traditional methods. Advanced AI methods, such as generative models and reinforcement learning, are being applied to design new molecules with desired properties, improving drug efficacy and enabling drug repurposing. AI also aids in predicting pharmacokinetics, toxicity, and drug-target interactions, improving safety profiles and reducing clinical trial failures. In clinical development, AI helps personalize treatment plans by evaluating patient data, optimizing clinical trial procedures, patient recruitment, and trial design. Despite challenges like data quality and regulatory concerns, AI holds the potential to revolutionize drug development, enabling faster, more effective treatments for patients.

INTRODUCTION: Drug development involves the comprehensive process of bringing a new drug molecule into clinical use. In its broadest sense, it covers all stages, from fundamental research focused on identifying suitable molecular targets to large-scale Phase III clinical trials that facilitate the drug's commercial launch, along with post-market pharmacovigilance and studies on drug repurposing [1].

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The drug development process includes identifying and rigorously testing chemical entities with potential as therapeutic agents, and it is time-consuming as well as costly [2]. It is expensive because high cost associated with R&D and clinical trials. On an average, it takes approximately 12 to 15 years for bringing a new drug molecule to the market for patient treatment.

The rate of drug production in the pharmaceutical industry is still on the decline. This tendency can be attributed to a number of factors, such as the existing saturation of the market, the challenges of introducing novel chemical matter through a convoluted approvals procedure, and the willingness-to-pay in both developed and developing countries.

The inherent difficulty of transferring the drug development process from basic science to early clinical trials will be the main topic of discussion here. More information on a variety of topics related to the field is available to scientists now than ever before, greatly exceeding their capacity to appropriately interpret and incorporate into their own workflows and research goals [3]. To overcome these challenges, researchers globally have increasingly adopted computational methods such as virtual screening (VS) and molecular docking, commonly known as traditional approaches. Nevertheless, these techniques also face challenges, including problems with accuracy and efficiency [4]. As a result, there is a growing interest in adopting innovative techniques that can effectively address the challenges faced by traditional computational methods. Artificial intelligence (AI), including deep learning (DL) and machine learning (ML) algorithms, has emerged as a potential solution to overcome the obstacles in drug design and discovery [5].

AI, Machine Learning, and Natural Language Process (NLP): AI is a branch of computer science that uses math, logic, and cognitive science to simulate human behavior. The integration of AI into the healthcare industry can be summarized as the application of techniques that allow computers to imitate human behavior. It includes machine learning (ML) and natural language processing (NLP). Further subset of ML is deep learning (DL). ML uses statistical methods to enable systems to learn independently, without explicit programming. It is divided into three types: supervised, unsupervised, and reinforcement learning. Supervised learning builds predictive models using input and output data, with methods like classification (for disease diagnosis) and regression (for predicting drug efficacy and ADMET properties) [6]. Unsupervised learning includes feature-finding and clustering techniques that categorize and analyze data exclusively from input data [7]. Reinforcement learning is a type of machine learning used in complex environments to optimize decision-making through trial and error, based on feedback. While similar to supervised learning in its goal of improving decisions, it differs in its learning approach [8].

Deep learning (DL) is a subset of machine learning that excels in generalization, feature extraction, and end-to-end learning. In DL, output is derived directly from input during training, with the model refined through iterations based on prediction errors. A deep neural network (DNN) is a feed-forward network with interconnected input, hidden, and output layers, using multiple neurons to model complex, nonlinear relationships and learn features from input data [9].

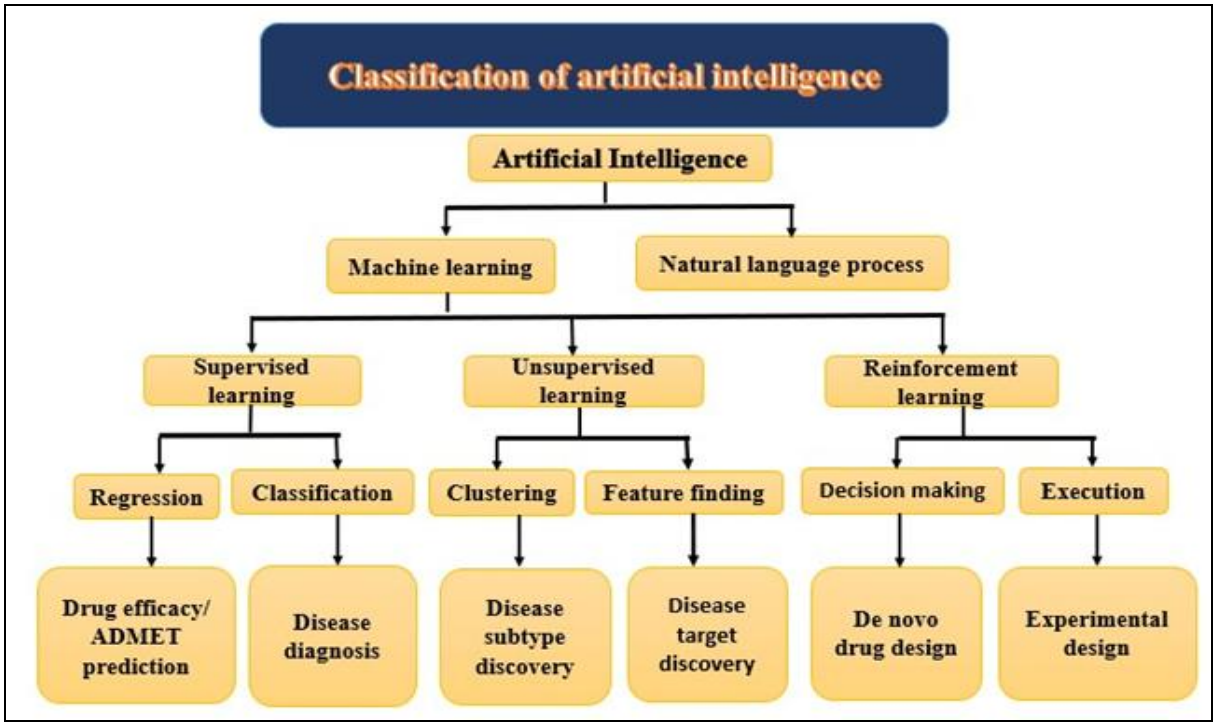

FIG. 1: CLASSIFICATION OF ARTIFICIAL INTELLIGENCE

Second class of AI is natural language processing (NLP) techniques that enhance and augment organized medical data by extracting information from unstructured sources like clinical notes and medical journals. The goal of NLP processes is to convert texts into structured data that is machine-readable so that ML approaches can analyze them [10].

History of AI: The idea of using computers to mimic human behavior and intelligence was initially proposed by Turing six years prior, but McCarthy first defined artificial intelligence (AI) in 1956 as "the science and engineering of making intelligent machines [11]." John Mc Carthy, an American computer scientist was called the father of Artificial Intelligence.

TABLE 1: A BRIEF HISTORY OF AI DEVELOPMENT

Year	Development
1943	Walter Pitts and Warren McCulloch proposed a model of artificial neurons, it was the first study to be acknowledged as artificial intelligence [3]
1949	Donald Hebb proposed a rule for adjusting the connection strength between neurons, which is referred to as Hebbian learning [12]
1950	Alan Turing's work, "Computing Machinery and Intelligence," introduced the idea of a "universal machine" that is able to act intelligently [12]
1955	Allen Newell and Herbert A. Simon developed the first artificial intelligence program, known as the "Logic Theorist." This program was able to prove 38 out of 52 mathematical theorems and even discovered new and more elegant proofs for some of them [13]
1956	The term AI was first used by American computer scientist John McCarthy during the Dartmouth conference, signifying the emergence of AI as an academic discipline [14]
1966	Joseph Weizenbaum developed the first chatbot, known as ELIZA [12]
1972	The first intelligent humanoid robot, known as WABOT-1, was constructed in Japan [15]
1975	The MYCIN system, created by Edward Shortliffe, showcased the use of expert systems for medical diagnosis by employing a rule-based approach [12]
1982	The R1/XCON system, developed by Douglas Lenat and Randal Davis, was a significant expert system used for configuring computer systems, demonstrating the effectiveness of rule-based reasoning [16]
1983	The CYC project, spearheaded by Douglas Lenat, aimed to develop a comprehensive knowledge base that includes common-sense reasoning and understanding [15]
1988	The Backpropagation algorithm, introduced by Paul Werbos, allowed for the efficient training of multi-layer neural networks [17]
1997	AI's ability to handle complex strategy games was demonstrated when IBM's Deep Blue defeated world chess champion Garry Kasparov in a six-game encounter [15]
1998	Yann LeCun et al developed the LeNet-5 architecture, which revolutionized computer vision and became a foundational model for image recognition applications [17]
2002	AI made its first entry into the home with the Roomba, a robotic vacuum cleaner [12]
2006	AI had entered the business world, with companies such as Facebook, Twitter, and Netflix beginning to implement AI technologies [12]
2009	The ImageNet project, spearheaded by Fei-Fei Li, created a large-scale dataset and benchmarks that facilitated the training of deep convolutional neural networks for image classification [17]
2011	In 2011, IBM's AI system Watson triumphed over human champions on the game show Jeopardy, showcasing its capabilities in natural language processing and knowledge retrieval [18]
2012	The AlexNet architecture, created by Krizhevsky, Sutskever, and Hinton, transformed image classification tasks and showcased the effectiveness of deep learning using GPUs [3]
2016	AlphaGo, created by DeepMind, triumphed over world champion Go player Lee Sedol, showcasing significant progress in machine learning and reinforcement learning [16]
2017	The Transformer model, presented by Vaswani *et al.*, transformed natural language processing tasks by allowing for efficient attention-based sequence-to-sequence modelling [18]
2018	Devin et al. developed BERT (Bidirectional Encoder Representations from Transformers), which achieved remarkable results in handling various natural language tasks, including question answering and sentiment analysis, across multiple languages [18]
2019	OpenAI's AlphaStar triumphed over professional players in StarCraft II, demonstrating the capabilities of reinforcement learning in complex real-time strategy games [3]
2021	For predicting the 3D protein structure, AlphaFold wins the CASP competition [17]
2022	The IEEE Global Initiative on Ethics of Autonomous and Intelligent Systems, the Partnership on AI, OpenAI's Charter, and other organizations [15]
2023	ChatGPT debuts, generating considerable debate [17]

Drug Development Process: The FDA defines the drug development process as consisting of four stages: (i) drug discovery, which involves identifying new therapeutic agents by understanding disease mechanisms; (ii) preclinical research, where laboratory and animal testing are conducted to assess the safety of new drug targets; (iii) clinical research, which includes several phases of human clinical trials to evaluate the drug's safety and effectiveness; and (iv) post-marketing research, focusing on comparative effectiveness studies and pharmacosurveillance to monitor the drug's performance after it reaches the market.

The drug development process begins by collecting data from computational modeling, high-throughput screening, and research. Researchers use inductive and deductive reasoning to identify potential drug compounds. Automation of steps like virtual screening and *in-silico* synthesis improves efficiency and accuracy, predicting toxicity and effectiveness without biochemical testing [6]. The drug development process begins by identifying a hit compound for optimization. High-throughput screening selects hits based on statistical analysis or inhibition thresholds, while fragment-based screening adjusts activity by molecular size to ensure potency and suitability [19]. Once a lead compound is identified, its efficacy and safety are evaluated in animal models. Further preclinical research assesses pharmacokinetics and toxicity. If results are promising, an Investigational New Drug (IND) application is submitted to the FDA for approval to begin human clinical trials. Clinical trials proceed in four phases: Phase 1 focuses on safety and dosage; Phase 2 evaluates efficacy and side effects; Phase 3 confirms efficacy in a larger population; and Phase 4, or post-marketing surveillance, tracks long-term effects. Before Phase 4, a New Drug Application (NDA) is submitted to the FDA for marketing approval.

AI in Drug Discovery and Drug Development: One of the biggest challenges in drug discovery is identifying effective and bioactive drug candidates from the vast chemical space of approximately 10^60 potential molecules, with 90% of candidates failing to advance past Phase II clinical trials or gain regulatory approval. However, these challenges can be mitigated by integrating AI-driven tools throughout the drug development process. AI helps design small molecules, optimize dosages, predict bioactive agents, analyze protein interactions and folding, perform virtual screening, conduct QSAR modeling, facilitate drug repurposing, and assess toxicity, bioactivity, and the mode of action of drug substances [5]. AI enhances outcomes in areas where traditional methods struggle, particularly when assessing complex properties like drug-likeness, which rely on the interplay of multiple factors.

Optimizing these compounds is a complex process, often supported by *in-silico* prediction techniques. Machine learning algorithms like Bayesian learning, Random Forests (RF), and support vector machines (SVM) are commonly employed to enhance the optimization process [20].

Further advancements in machine learning have improved drug discovery, especially through QSAR-based ligand-based virtual screening (LBVS). SVMs, Bayesian algorithms (including naïve Bayes), and Random Forests (RF) are key machine learning techniques in QSAR modeling, helping to identify potential therapeutic candidates by analyzing complex biological data and molecular interactions. These methods are advancing AI-driven tools in drug discovery [3]. While these models are excellent for predicting basic properties like logP and solubility, they struggle with more complex aspects like side effects and efficacy. Issues such as insufficient experimental validation, data errors, and small training sets often lead to overfitting, limited chemical space, and inaccurate predictions. Moreover, QSAR's assumption that structurally similar compounds will have similar activities is sometimes flawed, highlighting the need for more comprehensive models [21]. Combinatorial library screening includes both virtual and experimental methods. Virtual screening uses computational techniques like molecular docking, pharmacophore mapping, and QSAR to predict drug-target interactions. However, it has limitations, such as not fully replacing experimental screening and the challenge of synthesizing compounds. On the other hand, experimental methods like high-throughput screening (HTS) directly assess the biological activity of large numbers of molecules, providing more reliable results. Since, the 1990s, HTS has

revolutionized drug discovery by enabling fast screening of vast chemical libraries with minimal resources, often using robotics. This has reduced testing costs and contributed to big data, providing valuable insights into drug responses to specific targets [22].

AI in Virtual Screening: The advancement of virtual screening methods has slowed, limiting improvements in prediction accuracy. While virtual screening can identify marginally active ligands, optimizing them is challenging [3]. For initial compound selection, Richards and colleagues' new study demonstrates the efficacy of utilizing coarse-grained models. Virtual screening is broadly distinguish into two category: ligand based virtual screening (LBVS) and structured based virtual screening (SBVS).

Structure Based Virtual Screening: Structure-based virtual screening (SBVS) is a computational approach in drug development that identifies potential therapeutic candidates by predicting how small molecules (ligands) interact with target proteins (receptors) [23]. It selects compounds likely to bind to the protein and exhibit biological activity, based on the 3D structure of the target protein, which is often determined through techniques like X-ray crystallography, NMR spectroscopy, or computational methods such as AlphaFold [24, 25].

Ligand Based Virtual Screening: Ligand-based virtual screening (LBVS) relies on the structural and physicochemical properties of known active and inactive compounds, based on the principle that similar structures often have similar biological activities. AI-powered ligand-based methods are now the most widely used in virtual screening [3, 26]. In LBVS, the similarity between compounds in a library and known active compounds is assessed using molecular descriptors, which can be 1D and 2D (providing chemical properties and topological characteristics) or 3D (describing molecular fields, shape, volume, and pharmacophores). LBVS is particularly useful when the 3D structure of the target protein is unavailable, such as for G-protein-coupled receptors (GPCRs) or proteins in their apo form [23, 26, 27].

AI in Drug Design: Predicting 3D structure of target protein - Most pharmacological targets are proteins, and their structures are crucial for biological functions like cell signaling and enzymatic activity. While techniques such as NMR spectroscopy, cryo-EM, and X-ray crystallography can determine protein structures, they are costly and time-consuming, with only around 100,000 structures identified so far. To address this gap, new methods for determining protein structures are needed [28].

AI-based methods have become increasingly popular for predicting protein structures, driven by the availability of large protein datasets [29]. One early approach by Qian *et al.* (1988) used a neural network to predict protein secondary structures with a success rate of 64.3%. The complexity of protein structure prediction stems from the vast conformational space, often breaking down the problem into components like secondary (2°) structure, solvent-accessible surface area, backbone torsion angles and other one-dimensional (1D) structural properties [30]. Structure-based drug design (SBDD) relies on understanding protein structure to identify therapeutic compounds, but experimental methods to determine 3D structures are costly and time-consuming [31].

The most advanced tool for predicting protein 3D structures is DeepMind's AlphaFold, a neural network-based technology that achieves accuracy comparable to experimental methods [32]. The details of the algorithm and architecture of AlphaFold are outlined in the work by Senior *et al* [33]. To improve protein structure prediction, AlphaFold employs sophisticated neural networks that combine geometric, physical, and evolutionary constraints [32, 34]. De novo structure prediction aids structural genomics by filling in missing protein segments, identifying novel folds, and modeling proteins difficult to analyze with X-ray crystallography or NMR, providing early functional insights before experimental determination [35].

Predicting Drug Protein Interaction: In drug development, understanding how molecules interact with proteins in cellular networks is key to creating effective treatments [36]. Drug-protein interaction (DPI) prediction plays a crucial role in drug development, with two main approaches: machine learning and physics-based techniques. Physics-based methods, such as molecular docking,

model interactions at the atomic level using energy functions, but they are complex due to protein size and folding [37]. Protein folding, the process of predicting interactions from a linear 1D sequence to a 3D protein structure. Traditional 1D sequence methods struggle to capture the necessary 3D structural details for accurate DPI predictions [38]. Various methods have been developed to predict DPI, including docking simulations, literature mining, and techniques that integrate chemical, 3D structural and genomic data. Structural bioinformatics and protein cleavage site prediction are also used to improve prediction accuracy which is based on Chou's distorted key theory.[39] These methods aim to enhance the understanding of how drugs interact with proteins like enzymes, ion channels, and GPCRs. High-throughput techniques examining the genome, transcriptome, and proteome are further advancing our knowledge of these interactions [40]. Key drug-target protein interaction data has been collected from databases such as KEGG BRITE, BRENDA, SuperTarget, and DrugBank, which track interactions with enzymes, ion channels, GPCRs, and nuclear receptors [41].

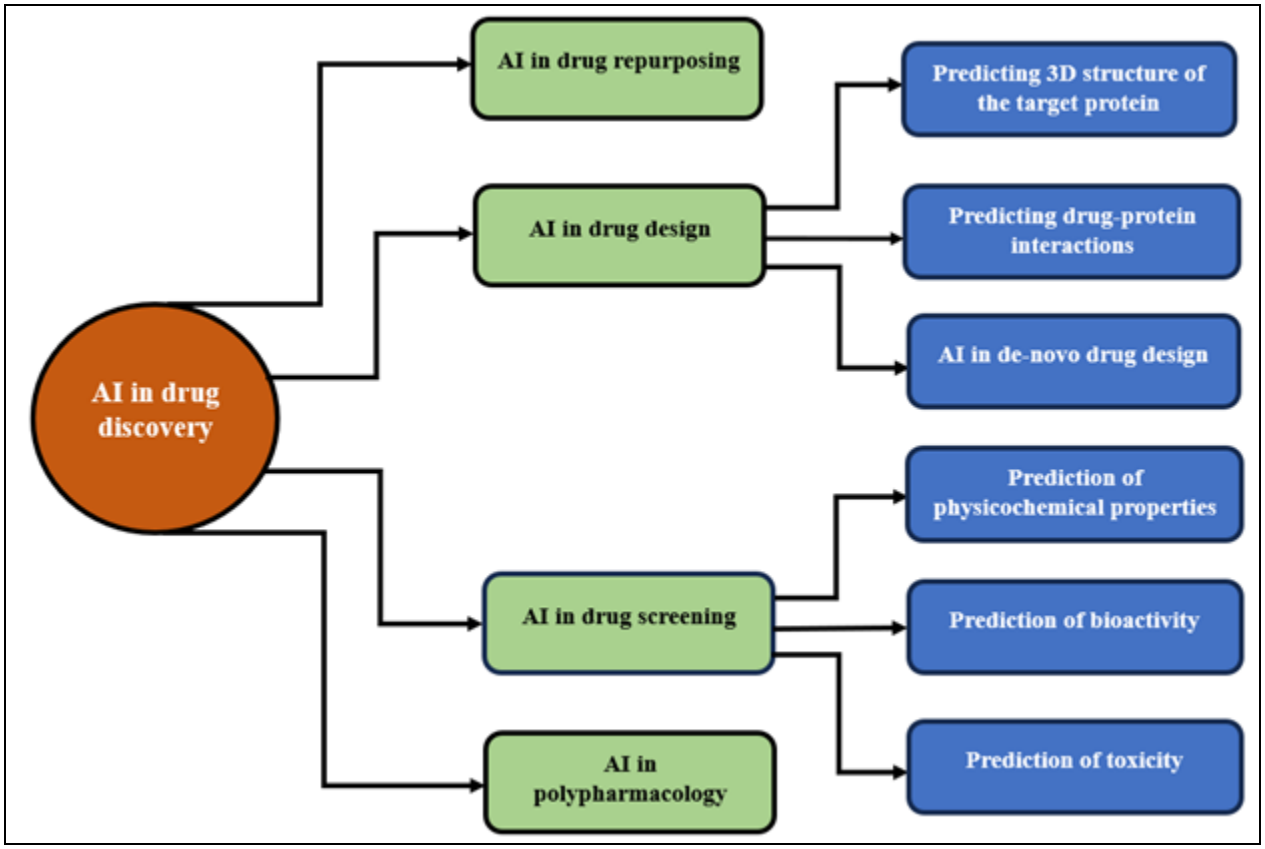

FIG. 2: AI IN DRUG DISCOVERY

AI in De Novo Drug Design: The term "de novo," meaning "from scratch", De novo drug design (DNDD) creates completely new chemical molecule, without using existing templates. It aims to explore uncharted chemical space and generate new compounds that meet specific biological requirements. Recently, deep reinforcement learning (DRL) has been integrated into DNDD, combining reinforcement learning and neural networks to enhance the design process [42]. Unlike methods like virtual screening, which optimize pre-existing molecules, de novo design creates entirely new chemical entities that do not exist in nature [43]. Key challenges in DNDD include navigating the vast chemical space and extracting desired properties. AI techniques, such as variational autoencoders (VAEs), generative adversarial networks (GANs), and recurrent neural networks (RNNs) with long short-term memory (LSTM) cells, have been employed to guide molecule design using molecular graphs or SMILES notation [44]. In DRL-based de novo drug design, an RNN is first trained on bioactive chemicals, such as those in the ChEMBL database, to predict molecular

sequences. The model is then used to generate new sequences, while a drug-design agent learns from reinforcement learning to optimize the drug design process. The agent's policy is refined over time to maximize the expected return, making this approach highly effective in generating novel, bioactive compounds [41, 45].

AI in Drug Screening: Advancements in AI, big data, and deep learning are transforming drug discovery by speeding up target identification, optimizing clinical trial success, and improving drug design efficiency. AI integration with high-throughput screening allows faster data processing, boosting the accuracy and success rate of drug development. Key collaborations, such as the UK's 100,000 Genomes Project and DeepMind's work with the Royal Free London NHS, showcase AI's growing impact on diagnostics, drug design, and treatment of rare diseases [46, 47].

Prediction of the Physicochemical Properties: Physicochemical properties like partition coefficients (logP), solubility (logS), melting and boiling points, vapor pressure, and bioconcentration factor (BCF) are crucial for understanding how chemicals behave in both the environment and biological systems. These properties influence exposure, toxicological risks, bioavailability, absorption, and persistence in the body and environment [48]. In medicinal chemistry, algorithms convert a molecule's IUPAC name into SMILES notation, representing its structure with ASCII strings, which can be visualized as 2D or 3D models. Using pattern-matching algorithms and databases like PubChem, known chemical structures can be identified, and new molecules can be designed [49].

Lipophilicity is a key factor in drug development, affecting pharmacokinetics, membrane permeability, and ADME behavior. Methods like logP, logD, and IAM algorithms estimate lipophilicity, while computational techniques such as group contribution methods, quantum chemistry, and QSAR models are also used. The average of predictions from models like XLOGP3, WLOGP, and iLOGP is often used to refine lipophilicity estimates [8]. Machine learning approaches in ADME research are helping to predict the pharmacokinetic properties of new drug candidates, optimizing molecules by forecasting bioavailability [50]. Prediction of bioactivity: AI has significantly advanced drug development, particularly in drug bioactivity prediction [34]. High-throughput screening (HTS) technologies, including mass spectrometry-based proteomics, genomics, and advanced chromatographic techniques, have accelerated drug discovery from natural products and enhanced biomedical insights [51]. The use of quantitative high-throughput screening (qHTS), which tests compounds at varying doses, has driven the development of activity-based approaches in drug discovery, generating valuable data for chemical activity forecasting. Over the past 15 years, more than half a million compounds have been screened, producing activity profiles that support biological activity-based modeling (BABM). Collections like LOPAC and the NCATS Pharmaceutical Collection (NPC) provide extensive datasets for training machine learning models [52].

In AI-driven drug discovery, molecules are represented by SMILES notation to form molecular graphs. Feature vectors are created based on bond attributes (such as bond type, stereochemistry) and atomic properties (such as bond count, atomic number). After refinement through message-passing algorithms, these feature vectors are fed into a neural network to predict the likelihood of a molecule having antibacterial properties [28].

Predicting toxicity: Recent online tools such as REACHacross2 and the Chemical In Vitro–In Vivo Profiling portal (CIIPro)enable automated extraction of data from databases like REACH and PubChem. Tools like Chembench and Charming support the development and sharing of curated toxicity data and QSAR models [53]. The U.S. EPA's distributed structure searchable toxicity (DSSTox) Database Network and the Vitic Toxicity Database, supported by pharmaceutical and chemical companies through Health and Environmental Science Institute (HESI) and managed by Lhasa Limited, store extensive toxicology data that can be re-analyzed using various techniques [54]. AI techniques, including DeepTox and PrOCTOR, are essential for predictive toxicology, helping assess toxicity risks in clinical trials and forecast the safety of new drugs. For example, Robledo-Cadena *et al.* (2020) was used PrOCTORto predict how NSAIDs affect the efficacy of cancer drugs like

doxorubicin and paclitaxel, while AI models helped explore new therapeutic indications for compounds targeting Type 2 diabetes and Parkinson's disease [5].

AI in Drug Repurposing: The high cost of drug development has led to a shift from the traditional "one disease, one target, one drug" model, making drug repurposing a more feasible strategy. By integrating genomic, proteomic, and metabolomic data, researchers can identify new targets for existing drugs [63].

In-silico methods using transcriptome data from various biological systems, along with deep learning, can predict a drug's potential for repurposing [6]. Drug repurposing often begins with unexpected findings, such as axitinib, initially developed for advanced renal cell carcinoma, showing activity against acute lymphoblastic leukemia (ALL) and chronic myeloid leukemia (CML) cells. Studies revealed axitinib binds strongly to the T315I-mutated BCR-ABL1protein, common in these cancers [55]. AI techniques like PREDICT, SLAMS, NetLapRLS, and DTINet combine data from multiple sources to identify potential drug repurposing opportunities [6].

AI in Polypharmacology: Polypharmacology, defined by the National Library of Medicine as the design or use of pharmaceutical agents that target multiple disease pathways, is integral to the development of multi-target treatments like CAR-T cells, bispecific monoclonal antibodies (BsMAb) and PROTACs [56]. Drug repurposing offers several advantages, including lower clinical failure rates, faster discovery, and reduced development costs by leveraging established safety profiles, thus avoiding redundant safety testing [55]. Various databases, such as ChemSpider, ZINC, PubChem, KEGG, ChEMBL, and DrugBank, provide extensive information on molecular pathways, structures, and biological activities, all of which can be explored by AI to develop polypharmacological agents. A prime example is the DeepDDI platform, which predicts drug-drug interactions and identifies alternative medications with minimal side effects for clinical use [6, 55].

TABLE 2: LIST OF AI BASED SOFTWARE AND TOOLS FOR DRUG DISCOVERY

AI based tools and software	Description
ChEMBL	ChEMBL is a curated database of bioactive compounds with drug-like properties [9]
PubChem	Chemical structures, identities, physical and chemical characteristics, and biological activities are all included in this open-access chemistry database [9, 29]
DrugBank	A comprehensive database containing information on drug targets and drug-related data [30]
DTC	The Drug Target Commons is a community-based, crowd sourced project that will collect, combine, annotate, and standardize quantitative bioactivity data on compound-target interactions from several database sources and scientific literature [29]
DeepChem	An open-source library offering a diverse set of tools and models for drug discovery, including deep learning algorithms for predicting molecular properties, conducting virtual screening, and enabling generative chemistry [57]
SMILES	The MOLBERT model applies the BERT architecture to SMILES notation for virtual screening [58]
SPIDR	Drug repurposing influenced by small-molecules peptides [5]
PubMed	The Biomedical Text Summarizer (BERT-based-sum) utilizes BERT and a hierarchical clustering algorithm to extract and summarize biomedical content [58]
DeepTox	Toxicological and biocompatible prediction [59]
Alphafold	A deep learning model for predicting protein structures [60]

AI in Clinical Trial: Clinical trial failures, which drive up costs and delays in drug development, are largely due to inefficient patient recruitment and monitoring.

AI and machine learning (ML) are being increasingly used to improve patient selection, predict treatment success, and reduce variability, thus enhancing trial efficiency and success rates [61]. AI helps identify patients based on biomarkers and supports drug discovery in areas such as drug targets, small molecules, biologics, vaccines, and repurposed drugs.

For example, IBM Watson uses AI to match patients with trials and predict outcomes, improving trial design and reducing costs. Ongoing AI advancements are expected to further optimize clinical trials and aid in personalized medicine development [61, 62].

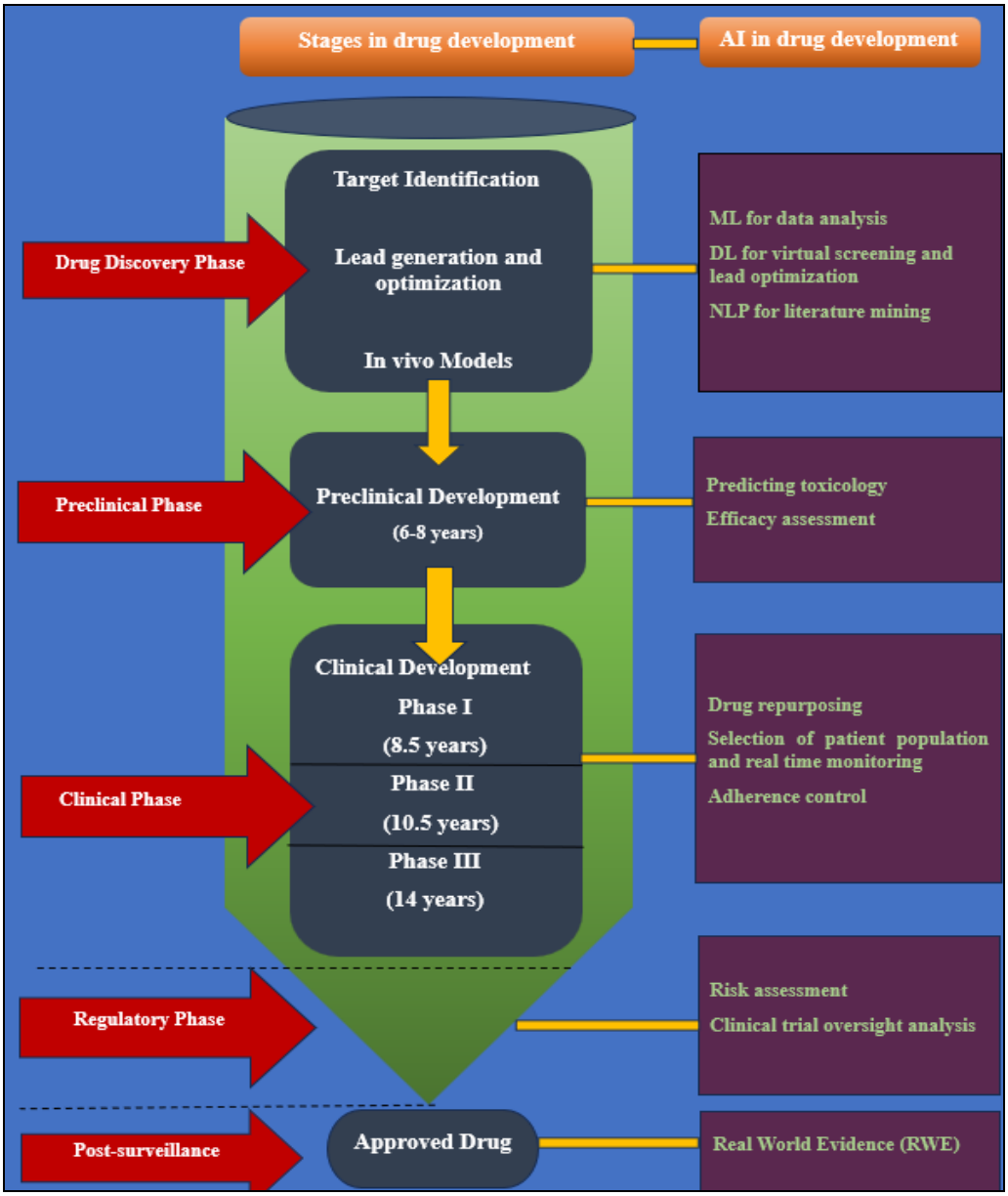

FIG. 3: AI IN DRUG DISCOVERY AND DRUG DEVELOPMENT PROCESS

AI in Pharmaceutical Manufacturing: Pharmaceutical formulation, which involves combining chemical compounds to create effective drugs, is a critical step in preclinical studies. AI is increasingly used to predict the properties of both solid and non-solid dosage forms, with a particular focus on solid forms like tablets. AI models help predict characteristics such as tensile strength, disintegration time, and brittleness based on factors like active pharmaceutical ingredient (API) properties, excipient types, and coating materials [63]. AI has enhanced the efficiency, accuracy, and cost-effectiveness of formulation development by analyzing experimental data to identify correlations between formulations, operational parameters, and quality attributes. This accelerates the optimization process, although if a formulation doesn't meet specific criteria (such as API loading, stability), it may need refinement, requiring multiple steps [64, 65]. Machine learning (ML), a subset of AI, is especially useful in predicting outcomes like drug stability by analyzing past data. With improved algorithms, faster computing, and more accessible tools, ML has become integral to pharmaceutical development, streamlining formulation processes and improving results [65].

CONCLUSION: Drug development is being revolutionized by AI, which increases cost-effectiveness, efficiency, and precision. It speeds up drug development, makes personalized treatment possible, improves predictive analytics,

and streamlines clinical trials. AI has many advantages, but there are also problems, such as data privacy and legal concerns. When AI and human knowledge work together, its full potential will be achieved, offering patients quicker and more efficient treatments.

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