Harnessing AI for Drug Discovery & Development: Transforming the Pharmaceutical Landscape

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Abstract:

This document explores the applications, benefits, and challenges of artificial intelligence (AI) in the pharmaceutical industry, particularly in drug discovery and formulation. AI methodologies, including machine learning (ML) and deep learning (DL), are revolutionizing stages from drug design to clinical trials by enhancing the predictability of drug interactions, toxicology, and efficacy. Key AI applications cover structure-based and ligand-based virtual screening, target protein structure prediction, and de novo drug design. Furthermore, AI models improve drug repurposing, predict adverse drug reactions, and optimize clinical trial selection, addressing cost, time, and resource inefficiencies. Despite its transformative impact, AI implementation faces challenges in data quality, interpretability, and cost. The future of AI in pharma emphasizes refining data-driven methods, enhancing algorithm accuracy, and integrating human expertise.

Keywords: Machine Learning, Drug Discovery,Virtual Screening, Drug Repurposing, Toxicology, Clinical Trials, Predictive Models.

1. Introduction

Artificial Intelligence (AI) has revolutionized the pharmaceutical industry, playing a crucial role in various aspects of healthcare. Many pharmaceutical companies face significant challenges in drug discovery and development due to limited research resources and high costs. AI has emerged as a transformative solution, enhancing efficiency in drug development[1].

AI is a branch of computer science that replicates human-like intelligence, enabling advanced data analysis. It operates through specialized algorithms and incorporates machine learning (ML) and deep learning (DL). ML, a core AI technique, allows machines to learn from existing data using statistical methods and make predictions. It is further divided into supervised, unsupervised, and reinforcement learning. DL, a subset of ML, employs multi-layered artificial neural networks (ANNs) to replicate human brain functions, making it highly effective for processing complex and high-dimensional data. Due to its speed and cost-effectiveness, ML is transforming various stages of drug discovery, including target identification, de novo drug design, and drug repurposing.Several DL-based open-source tools, such as DeepDTAF and DeepAffinity, have been developed to predict drug–target interaction (DTI) binding affinities, streamlining the search for new drugs. Consequently, major pharmaceutical companies, including Sanofi (France), Merck (Germany), Takeda (Japan), and Genentech (USA), have collaborated with AI firms to accelerate drug development[2].

Given the growing impact of ML in the pharmaceutical sector, this article explores recent advancements, opportunities, and challenges in ML-driven drug discovery. It first provides an updated overview of ML applications across different drug discovery stages, such as drug design, screening, repurposing, and chemical synthesis. It then examines the potential of advanced Transformer-based models in drug discovery. Finally, the challenges and future directions of ML in this field are discussed.

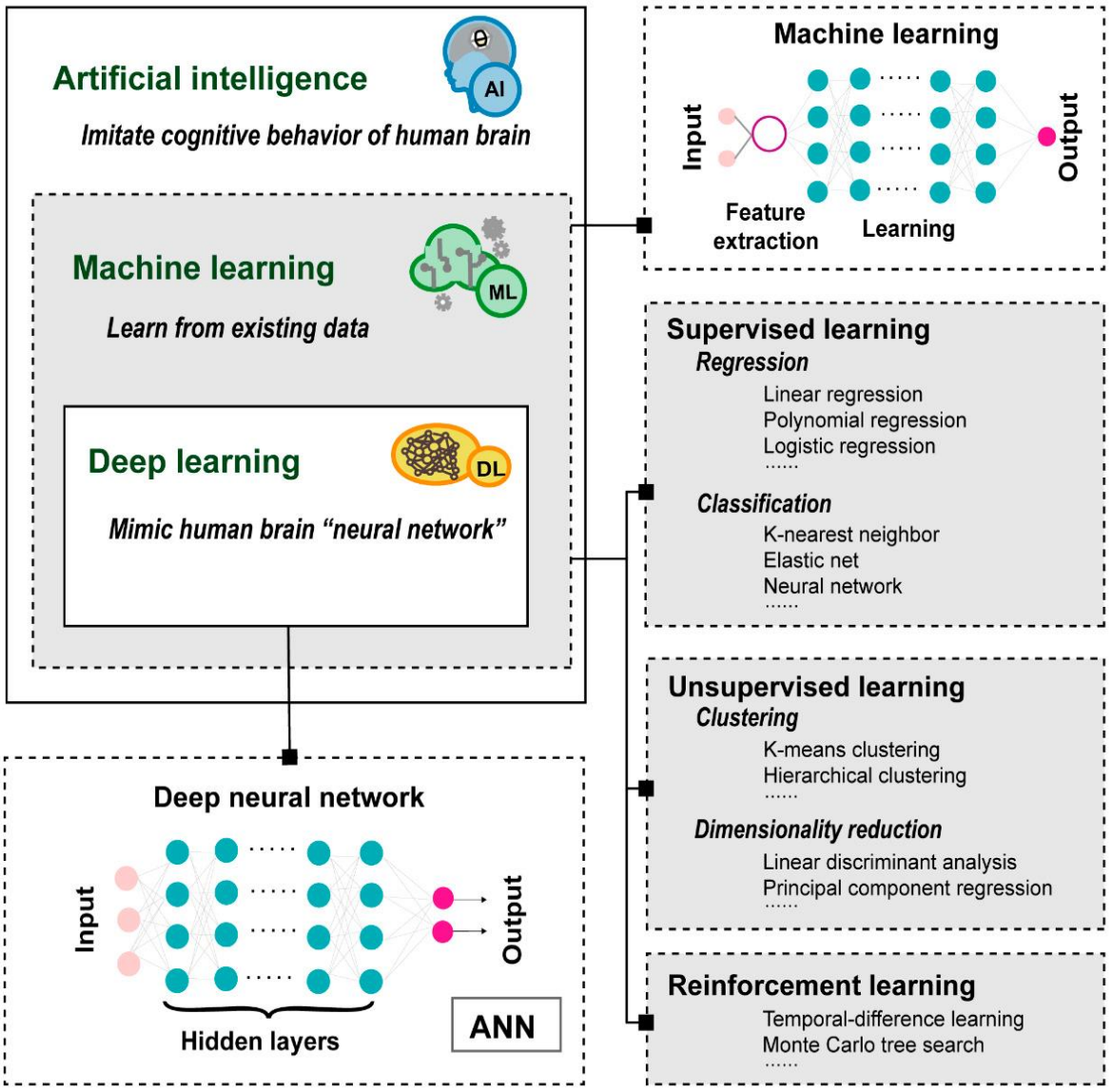

Fig: 1 Introduction diagram of artificial intelligence and its subfields: machine learning and deep learning[2].

Applications of ML in Drug Discovery

The discovery of effective new drugs is a lengthy and highly complex phase of drug development[2]. Leveraging its ability to analyze data, identify patterns, and make informed decisions, machine learning (ML) has become a powerful tool across various stages of drug discovery, including drug design, screening, repurposing, and selecting patient populations for clinical trials. Additionally, significant efforts are being made to create models, tools, software, and databases built on ML algorithms to address the inefficiencies and uncertainties associated with traditional drug development processes.

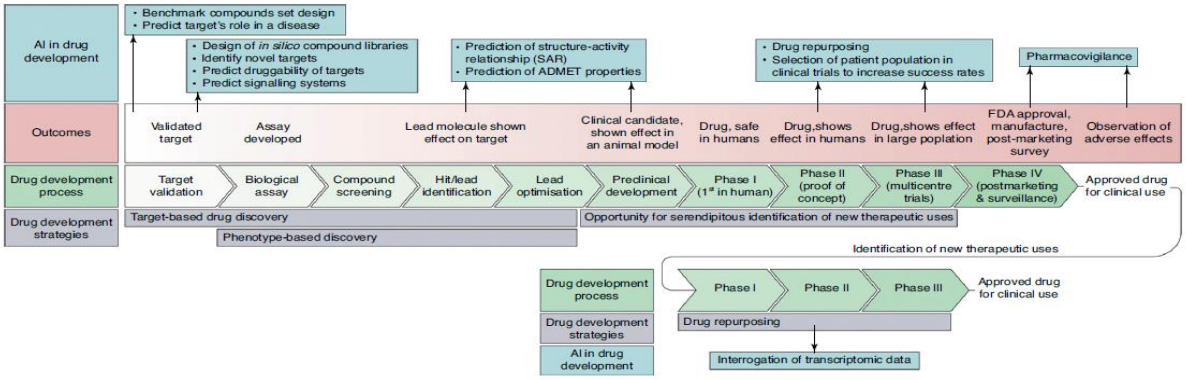

Fig: 2 Drug discovery and development[3]

2. Applications of AI in Dosage Form Designs

The human body is divided into compartments that influence drug delivery, with biological membranes playing a key role[4]. Drug permeation, affected by the delivery method and administration route, is essential for effective monitoring. For oral drugs, absorption through the intestinal or gastric epithelium ensures distribution to the bloodstream. While passive diffusion depends on molecular properties, active permeation involves complex biological interactions. AI-driven models improve predictions of drug distribution and pharmacokinetics, though some discrepancies with real studies remain. By refining simulations and analyzing interactions, AI enhances understanding of drug disposition, toxicity, and delivery, aiding preclinical evaluations.

2.1. Benefits of AI technology

AI is a complicated domain. It combines computer science,mathematics, and other fieldsin a complex way[5].

- **Error Reduction**:
  - AI minimizes errors and improves accuracy.
  - Ideal for space exploration due to resilience to harsh conditions.
- **Difficult Exploration**:
  - Useful in petroleum exploration and ocean studies.
  - Robots handle demanding tasks without fatigue.
- **Routine Implementations[6]:**
  - Enhances tools like GPS for navigation.
  - Enables spelling corrections and predictive text in devices.

- **Digital Assistants**:
    - Avatars reduce dependency on human resources.
    - Logical decision-making without emotional interference.
- **Repetitive Jobs**:
    - Machines excel in multitasking and handling risky tasks.
    - Faster and more efficient than humans.
- **No Breaks**:
    - Machines operate continuously without requiring rest.
- **Aids and Assistance**:
    - Provide 24/7 support to the elderly or disabled.
    - Enhance education and security (e.g., alerts for robberies, fires, weather).

- **Enhancing Technological Progress**:
    - AI drives global cutting-edge advancements.
    - Generates advanced computational modeling programs.
    - Supports the development of innovative drug delivery formulations.

2.2. Challenges of AI[5]

- **High Costs**:
    - Designing, maintaining, and repairing AI systems is expensive.
    - Requires time-intensive research, regular updates, and costly reinstallations.
- **No Human Duplication**:
    - AI robots lack human emotional intelligence and subjective judgment.
    - Cannot handle unfamiliar problems effectively.
- **No Experience-Based Improvement**:
    - Unlike humans, AI cannot improve through experience.
    - Unable to evaluate or differentiate human efforts.
- **Lack of Creativity**:
    - AI lacks emotional intelligence and the ability to think creatively.
    - Machines cannot replicate human sensory or innovative capabilities.

- **Job Displacement**:
    - Widespread AI adoption may lead to unemployment.
    - Reduced productivity and creativity in the workforce due to job loss.

3. Applications of ML in Drug Design

Prediction of the Target Protein Structure

Proteins are vital to numerous biological processes;their dysfunction can lead to diseases[8]. Designing small-molecule drugs for disease treatment often involves understanding the 3D chemical environment of ligand-binding sites in target proteins, making accurate protein structure prediction crucial for drug discovery. Traditionally, homology modeling has been used, relying on known protein templates[9]. However, machine learning (ML) approaches, such as AlphaFold by DeepMind, have demonstrated superior accuracy and efficiency. Using deep neural networks, **AlphaFold** predicts 3D protein structures by analyzing amino acid distances and peptide bond angles, revolutionizing protein structure prediction and advancing drug discovery[10]. Despite these advancements, challenges remain due to proteins ability to form multiple coexisting structures and undergo environmental changes[11]. ML approaches thus hold significant potential to deepen our understanding of protein structures and enhance drug discovery efforts.

Structure-based virtual screening (VS)

Structure-based virtual screening (SBVS) is a critical method in drug development that leverages 3D structures of drug targets and compounds, typically obtained from X-ray crystallography or nuclear magnetic resonance (NMR)[12,13]. The process involves molecular docking, where a ligand is virtually docked into a receptor's binding site, followed by the calculation of binding affinity using mathematical scoring functions. Popular docking tools include AutoDock, Glide, and DOCK[14-16].

Recently, AI algorithms have been employed to enhance scoring functions and improve accuracy over traditional methods. Techniques such as naïve Bayes, support vector machines (SVM), random forests (RF), feed-forward artificial neural networks (ANNs), and deep neural networks (DNNs) are utilized to refine predictions[17-20]. For instance, RF-Score has significantly improved binding affinity predictions, and ALADDIN, an integrated ML and docking approach, has addressed challenges like protein flexibility and solvation in VEGFR2, p38α MAPK, and GCR [21].

Deep learning (DL), a subset of ML, is also making strides in drug design.ML methods (e.g., RF, SVM) identified P-glycoprotein inhibitors from ChEMBL and resolved naïve Bayesian model issues for 20 protein kinases, with RF showing superior performance[19]. DeepVS, based on convolutional neural networks (CNNs), achieved high accuracy with its approach[22].

Although AI application in SBVS shows great promise, results are contingent on factors like dataset quality, model selection, and parameter definitions.

Ligand-based virtual screening

Ligand-based virtual screening (LBVS) is a valuable approach when the 3D structure of the target protein is unavailable, leveraging the principle that structurally similar compounds exhibit similar biological effects[17,23]. AI techniques such as artificial neural networks (ANNs), random forests (RF), support vector machines (SVM), and deep neural networks (DNNs) have advanced LBVS, particularly in quantitative structure-activity relationship (QSAR) modeling[23,24].ANN outperformed MLR (R^2 training: 0.8520 vs. 0.4049) in predicting the relationship between physicochemical properties and output descriptors for a dataset of 90 pyridinylimidazole-based inhibitors of p38R MAP kinases[25], whileSix methods (e.g., partial derivatives(PaD- most stable that has be concluded by researchers), weights, perturbation, and ranking analysis) were applied to optimize ANN architectures, revealing quantum mechanical molecular descriptors' relationship with the Trolox-equivalent antioxidant capacity of 33 flavonoids[26].Variants like feed-forward backpropagation (BP-NN) networks have been effective in modeling inhibitory activities of pyridinone derivatives against HIV-1 reverse transcriptase for pIC50[27]. DNNs have shown exceptional promise for large datasets(ChEMBL) outperforming RF in predicting EGFR inhibitors and screening compound libraries(PubChem,ChemDiv)[28]. LS-SVM and genetic algorithm-MLR have accurately predicted IC50 values of poly ADP-ribose polymerase-1inhibitors for breast cancer[29], while RF has effectively assessed the toxicity of nano-TiO2[30]. Comparative studies reveal that XGBoost is the best classifier for histone deacetylase-3 inhibitors, and Sequential Minimal Optimization (SMO) excels in classifying HIV-1 integrase inhibitors. These examples highlight how AI-driven LBVS methods, combined with large datasets, are significantly advancing drug discovery and development[31,32].

De Novo Drug Design

De novo drug design involves creating novel drug molecules from scratch using computational methods, without relying on existing compounds. Traditional methods, such as fragment-based approaches, often result in molecules with poor drug metabolism, pharmacokinetics, and synthesis practicality[33,34]. To overcome these limitations, machine learning (ML) techniques have been increasingly applied. Notable examples include **PaccMannRL**, which combines variational auto-encoders (VAE) and reinforcement learning to design anti-cancer molecules based on transcriptomic data[35], and **druGAN**, which uses a deep generative adversarial auto-encoder (AAE) to generate anticancer molecules[36]. **MedGAN**, based on a Wasserstein GAN and graph convolutional network (GCN), has demonstrated success in generating novel quinoline-scaffold molecules, with 25% of generated compounds being effective and unique[37]. To address the challenge of synthesizing these molecules, **SCScore**, developed by Coley et al., uses neural networks to assess the synthetic complexity of generated compounds[38]. These ML-based approaches are transforming de novo drug design, making it more efficient in discovering new therapeutic molecules.

Designing compounds using de novo synthesis with tools like DruGAN involves several key steps. DruGAN (Drug Generative Adversarial Network) is a machine learning approach that uses GANs (Generative Adversarial Networks) to generate novel drug-like compounds. Here's a brief overview of the procedure:

1. **Data Collection and Preparation**:
    - **Gather Data**: Collect a dataset of known drug-like compounds, including their chemical structures and biological activities.
    - **Preprocess Data**: Prepare the data for training, which often involves encoding chemical structures into a format suitable for machine learning, such as SMILES strings or molecular fingerprints.
2. **Model Training**:
    - **GAN Architecture**: DruGAN typically involves a GAN architecture with a generator and a discriminator. The generator creates new chemical structures, while the discriminator evaluates their quality based on how closely they resemble real drug-like compounds.
    - **Training**: Train the GAN using the pre-processed data. The generator learns to produce compounds that are increasingly similar to the training data, while the discriminator improves its ability to distinguish between real and generated compounds.
3. **Compound Generation**:
    - **Generate Compounds**: Once trained, use the generator to produce new chemical structures. These structures are designed to be novel and potentially drug-like.
    - **Optimization**: Depending on the application, you might need to optimize the generated compounds for specific properties or activities.
4. **Evaluation**:
    - **In Silico Testing**: Evaluate the generated compounds using computational methods to predict their drug-like properties and potential biological activities.
    - **Experimental Validation**: Optionally, synthesize and test the most promising compounds experimentally to validate their efficacy and safety.
5. **Iteration**:
    - Refine Use feedback from evaluations to refine the model. This might involve retraining the GAN with additional data or adjusting the model parameters.

Prediction of the Physicochemical Properties

Physicochemical properties, such as solubility, ionization degree, partition coefficient, permeability, and stability, are crucial in determining a drug's behavior in biological systems and the environment. These properties influence factors like bioavailability, absorption, and potential health risks, making their prediction an essential step in drug screening[39,40]. To aid in this process, multiple machine learning (ML) tools have been developed to predict these properties, helping identify promising drug candidates for further development.

One notable ML-based tool is **SolTranNet**, a molecule attention Transformer developed by Francoeur et al. to predict aqueous solubility from the SMILES representation of drug molecules[41]. SolTranNet has proven effective as a classifier for filtering insoluble compounds, achieving a sensitivity of 0.948 on the Challenge to Predict Aqueous Solubility (SC2) datasets. This performance is competitive with other existing methods[40].

Determination of Physicochemical Properties of Compounds Using SolTranNet:

1. **Installation and Setup**:
    - Install SolTranNet and its dependencies, ensuring the required machine learning libraries and tools are configured.
2. **Data Preparation**:
    - Prepare the input data, typically in the form of SMILES strings or molecular descriptors of the compounds.
    - Format the data according to SolTranNet requirements (e.g., CSV files with appropriate columns).
3. **Model Training (if required)**:
    - If a pre-trained model is not available, train SolTranNet using a dataset with known physicochemical properties (e.g., solubility, logP, or pKa).
    - Ensure the dataset covers a diverse range of chemical structures for robust predictions.
4. **Prediction**:
    - Input the compound data (SMILES or descriptors) into SolTranNet.
    - Run the model to predict desired physicochemical properties, such as solubility, lipophilicity, or partition coefficients.
5. **Evaluation and Refinement**:
    - Compare predictions with experimental or literature data (if available) to validate the model's accuracy.

- Refine the model by incorporating additional data or adjusting parameters if predictions deviate significantly.

6. **Output and Analysis**:
   - Analyze the predicted physicochemical properties to assess the compound's drug-likeness, solubility, or other relevant features.
   - Use these insights for further compound development or optimization.

Additionally, Zang et al. developed a **quantitative structure–property relationship (QSPR) workflow** that uses molecular fingerprints and four ML algorithms to predict six physicochemical properties of environmental chemicals. These properties include water solubility, octanol–water partition coefficient, melting point, boiling point, bioconcentration factor, and vapor pressure.

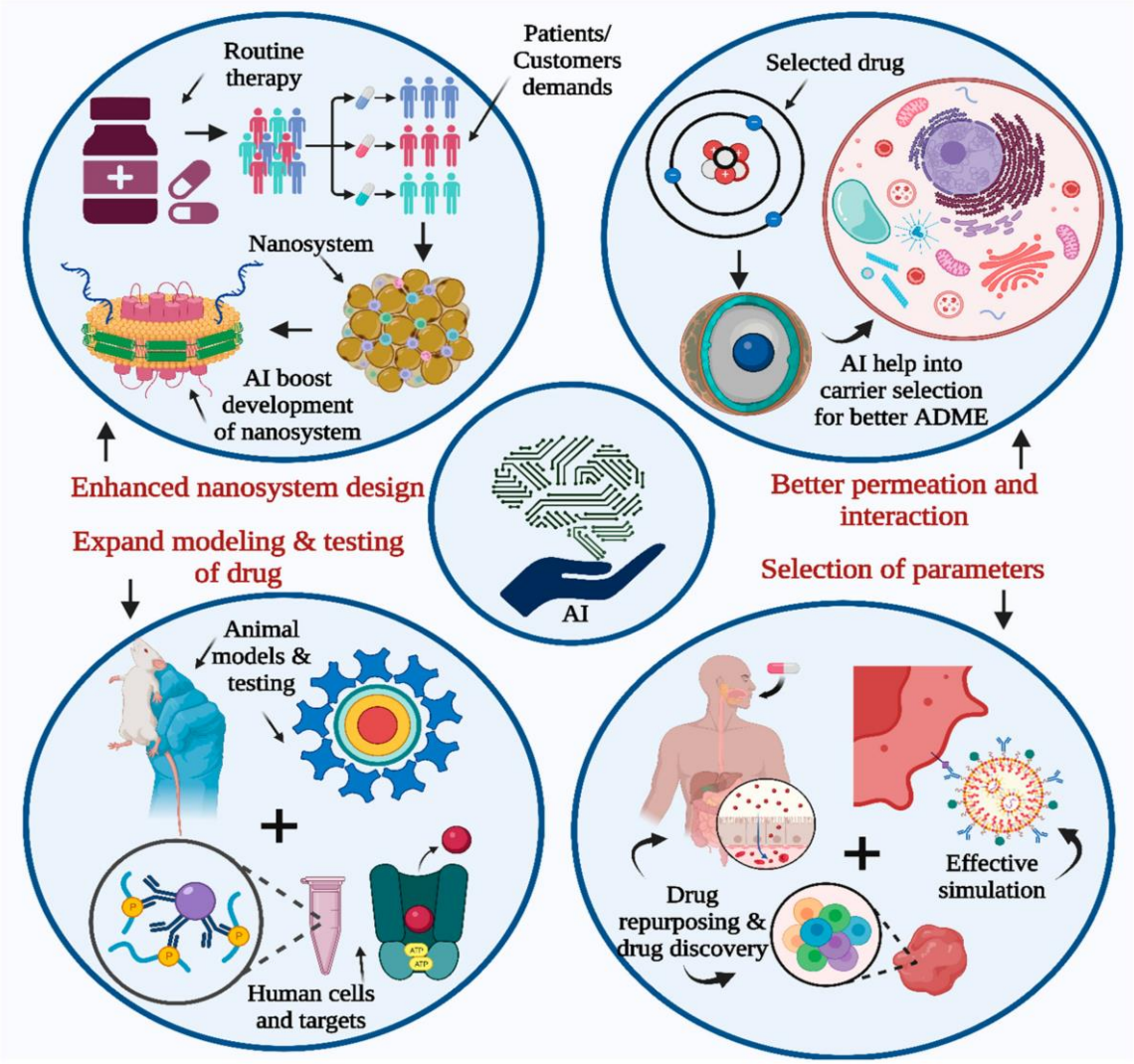

Fig: 3 AI enhances drug development by improving nano system design, drug testing models, parameter selection, and understanding drug interactions with human cells[4].

Prediction of the ADME/T Properties

Assessing absorption, distribution, metabolism, excretion, and toxicity (ADME/T) properties is crucial in drug discovery to evaluate a compound's behavior and safety in the human body. ADME/T failures often lead to late-stage drug development failures or withdrawal of approved drugs. Consequently, these properties are critical molecular filters in early drug screening[42,43]. Various machine learning (ML) tools have been developed to predict ADME/T properties with high accuracy. For example, **ADMETboost**, a web server by Tian et al., uses the XGBoost model to predict properties such as Caco2 permeability, blood-brain barrier (BBB) penetration, and CYP2C9 inhibition,CL-Hepa and hERG achieving top performance in the Therapeutics Data Commons ADMET benchmark,ranking first in 18 out of 22 tasks[44].Similarly, a **multitask autoencoder DNN** by Li et al., using data from 13,000 compounds, predicted inhibitors for five major CYP450 isoforms(1A2, 2C9,2C19, 2D6 and 3A4) with 86.4% accuracy in cross-validation and 88.7% on external datasets, outperforming traditional ML methods[45].

In toxicity prediction,The Tox21 Challenge focuses on creating predictive models for toxicity assessment using high-throughput screening data. Mayr et al. developed a deep learning pipeline, **DeepTox**, which outperformed traditional computational methods like naïve Bayes, random forest, and SVM in 10 out of 15 cases, showcasing its effectiveness in toxicity prediction[46]. These ML tools are significantly advancing the prediction of ADME/T properties, improving drug safety assessments and preclinical research.

Application of ML in Drug Repurposing

Drug repurposing, or repositioning, involves finding new uses for approved or investigational drugs, leveraging existing safety data to accelerate development and reduce costs[47]. Machine learning (ML) methods are increasingly applied to this process, with approaches broadly categorized into target-centered and disease-centered strategies[48].

In target-centered repurposing, network-based methods are used to discover new drug targets. For example, **deepDTnet**, developed by Zeng et al., employs autoencoder and Positive-Unlabeled matrix completion algorithms to identify new targets from a heterogeneous drug–gene–disease network, achieving an impressive AUC of 0.963[49]. Similarly, **DTINet** by Luo et al. combines network diffusion with dimensionality reduction to enhance drug–target interaction prediction, outperforming other methods with higher AUC and precision-recall (AUPR)scores like 5.7% and 5.9%[50].

Disease-centered approaches focus on identifying drug–disease relationships and are divided into similarity-based and network-based methods[51]. **MBiRW**, introduced by Luo et al., uses similarity measurements and a Bi-Random Walk algorithm to predict novel drug indications, achieving a high AUC of 0.917[52]. Additionally, **GDRnet**, developed by Doshi et al., utilizes a graph neural network to efficiently screen drugs and predict their therapeutic effects, integrating information from various biological networks[53].

These ML-based methods significantly advance drug repurposing, offering powerful tools to accelerate drug discovery and identify new therapeutic uses for existing drugs.

Role of AI in adverse drug reactions

AI significantly enhances pharmacovigilance, which encompasses monitoring, detecting, and preventing adverse drug reactions (ADRs). This field is crucial for ensuring drug safety through two main phases: evaluating drugs for adverse effects before market launch and monitoring post-marketing adverse events in the general population.

AI addresses challenges in pharmacovigilance by improving the handling of vast databases and reducing human error. Machine learning (ML) and deep learning (DL) techniques are central to this process. ML algorithms create models to predict ADRs by analyzing structured and unstructured data, thus enhancing efficiency and accuracy. DL techniques, such as those involving neural networks, excel in processing complex data, including images and speech, leading to more precise clinical outcomes[54].

Specific AI tools support these functions. **VigiBase**, for instance, manages a database of around 20 million adverse drug reports, while **VigiAccess** provides access to this data[55]. **VigiFlow** facilitates online data collection and analysis, **VigiGrade** assesses the clinical relevance of individual reports, and **VigiRank** detects statistical signals[56]. The WHO-UMC utilizes Bayesian Confidence Propagation Neural Network for clinical evaluations[57]. Despite these advancements, the economic costs associated with AI systems remain a concern.

Prediction of Protein–protein interactions

Protein–protein interactions (PPIs) are vital for various biological processes and are crucial targets in drug design. Machine learning (ML) methods have been employed to predict PPIs, with approaches broadly categorized into structure-based and sequence-based techniques[58]. Structure-based approaches use protein structural similarities to predict interactions. For instance, **IntPred**, a random forest-based tool, predicts protein–protein interface sites and has demonstrated strong performance with an accuracy of 0.811 and a Matthews' Correlation Coefficient (MCC) of 0.370[59]. Another example is **Struct2Graph**, a graph attention network (GAT)-based classifier that directly predicts PPIs from 3D protein structures, achieving near-perfect accuracy of 0.9989 on balanced datasets[60]. Sequence-based approaches, on the other hand, use protein sequence data to predict physical interactions[61]. **DeepPPI**, a deep neural network (DNN)-based tool, has shown excellent performance on S. cerevisiae dataset, with an accuracy of 0.925 and AUC of 0.9743. DeepPPI demonstrated superior predictive performance compared to existing methods by effectively learning useful features of protein pairs through layer-wise abstraction, as validated on core *S. cerevisiae*, *H. pylori*, and *H. sapiens* datasets[62].

DELPHI, a deep ensemble model, predicts PPI-binding sites using data from the Uniprot database. While sequence-based methods benefit from abundant protein sequence data, structure-based approaches are often limited by the availability and quality of protein

structures[63,42]. These ML tools are advancing our understanding of PPIs, which is critical for drug discovery and development.

Prediction of Drug–target interactions 2

Drug–target interactions (DTIs) are fundamental to the therapeutic effects of drugs, as they involve the interaction of drugs with specific target molecules like enzymes, receptors, and ion channels. Accurately predicting DTIs is crucial in drug design, but traditional experimental methods are often time-consuming and expensive. As a result, machine learning (ML) has become an increasingly popular approach for predicting DTIs, focusing on predicting binding sites, estimating binding affinity, and determining binding poses[64].

Binding sites, or binding pockets, are specific regions within a protein where interactions between the protein and a ligand (such as a drug molecule) occur. For instance, **DeepC-SeqSite**, a sequence-based method developed by Cui et al., uses a deep convolutional neural network (CNN) to predict protein–ligand binding residues[65]. This method outperformed several existing sequence-based and 3D-structure-based methods, including the leading COACH method[65]. Another example is **AGAT-PPIS**, proposed by Zhou et al., which uses an augmented graph attention network (GAT) to predict binding sites, achieving an 8% accuracy increase over the state-of-the-art method on benchmark tests[66].

Binding affinity refers to the strength of the interaction between a drug and its target. Various ML and deep learning (DL) tools have been developed to estimate binding affinity, such as **DEELIG**[67] and **GraphDelta**[68], which leverage these algorithms to determine DTIs' binding affinity.

Nguyen et al. developed a scoring function by combining random forest and CNN strategies to select the most relevant docking poses from GOLD, GLIDE, and Autodock Vina, improving ligand–target binding accuracy[69]. This approach helps in obtaining more accurate and effective ligand–target binding configurations.

Selection of population for clinical trails

AI in selection of a population for clinical trials an ideal AI tool to assist in clinical trials should recognise the disease in patients, identify the gene targets and predict the effect of the molecule designed as well as the on- and off-target effects. A novel AI platform called AiCure was also developed as a mobile application to measure medication adherence in a Phase II trial of subjects suffering from schizophrenia, where it was reported that **AiCure** increased adherence 25% compared with the traditional ‘modified directly observed therapy[70]. Patient selection for a clinical trial is a crucial process. Interrogating the relationship between human-relevant biomarkers and in vitro phenotypes affords a more predictable, quantifiable assessment of the uncertainty of therapeutic responses in a specific patient. The development of AI approaches to identify and predict human-relevant biomarkers of disease allows the recruitment of a specific patient population in Phase II and III clinical trials. The AI predictive modelling in selection of a patient population would increase the success rate in clinical trials[71, 72].

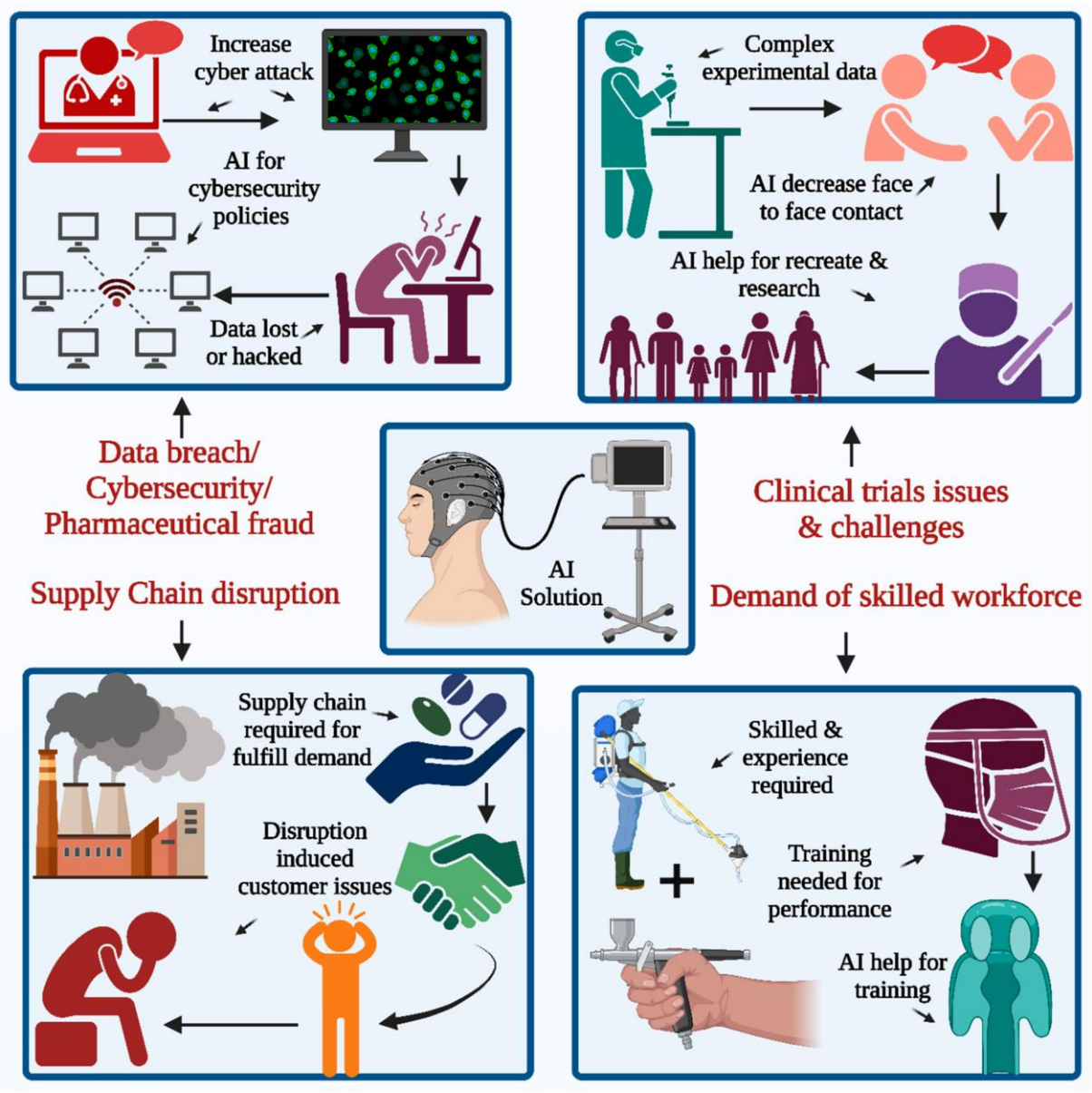

Fig: 4 An AI solution for the pharmaceutical industry must address workforce proficiency, supply chain disruptions, clinical trial challenges, and rising cybersecurity threats[4].

AI in Medical Devices

AI is revolutionizing medical devices by improving diagnostics, monitoring, treatment, and patient care. Advanced AI algorithms analyze medical imaging, including X-rays and MRIs, to aid in detecting diseases such as cancer and heart conditions. For example, AI-driven imaging enhances diagnostic precision by identifying cancerous lesions and ECG abnormalities.

AI has greatly progressed the field of medical devices, strengthening diagnosis, monitoring, treatment, and overall patient care. Below are key areas where AI is making a significant impact[4]:

- **Diagnostic Assistance:** AI analyzes medical imaging such as X-rays and CT scans to aid in diagnosing diseases like cancer. It detects cancerous lesions and ECG abnormalities, improving diagnostic accuracy for healthcare professionals.
- **Remote Monitoring:** AI-powered devices continuously track vital signs and health conditions, providing personalized care, especially for chronic diseases. AI alerts healthcare providers to any significant changes.
- **Wearable Devices:** AI integrates into wearables like smartwatches and fitness trackers to monitor heart rate, blood glucose levels, and other health parameters, offering actionable insights.
- **Prosthetics and Rehabilitation:** AI enhances prosthetics by enabling natural movement based on user intentions. It also supports rehabilitation by analyzing motion and providing feedback for improved recovery.
- **Surgical Assistance:** AI-driven robotic systems enhance precision in minimally invasive surgeries, offering real-time guidance using preoperative and intraoperative data.
- **Medication Management:** AI-powered devices, such as smart pill dispensers, assist in medication scheduling and dosage management, providing personalized recommendations.

Ex: Medtronic's Guardian Connect system integrates AI with continuous glucose monitoring, offering real-time insights for diabetes management. The Medtronic Sugar IQ app, developed with IBM Watson, analyzes glucose patterns, provides real-time guidance, and includes food logging to help users manage diabetes effectively.

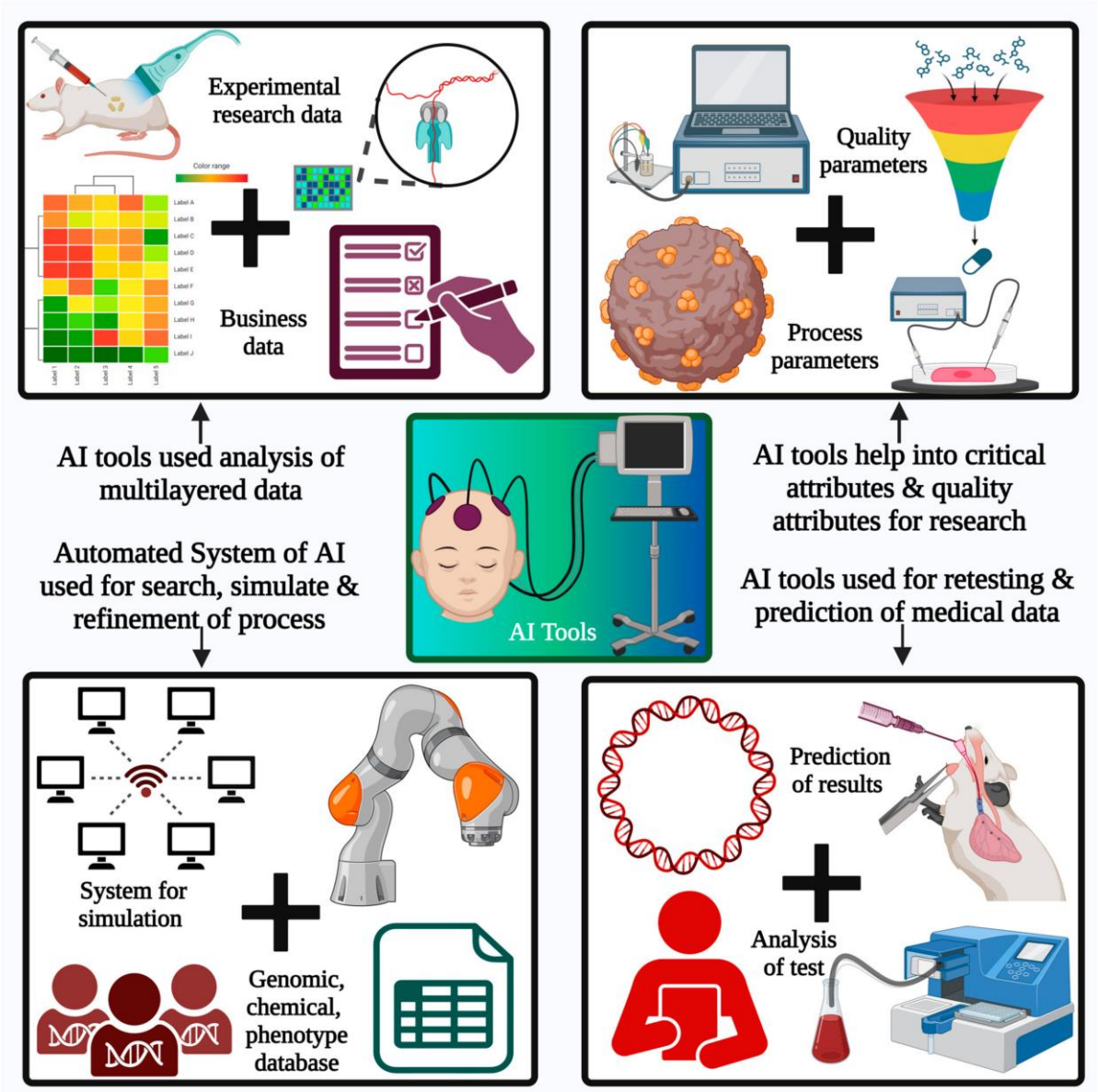

Fig: 6 AI tools in pharma analyze multilayered data, perform automated searches, and optimize drug models, predictionsusing diverse databases[4].

- Other applications include[7]

S.No.	Technologies	Description
1.	Analyze different test	▪ AI effectively interprets various medical imaging tests such as X-rays, ultrasounds, MRIs, and CT scans. ▪ It can assess disease progression and identify key contributing factors. ▪ Enables rapid sharing of patient information in emergencies, assisting doctors and surgeons. ▪ Efficiently processes, evaluates, validates, predicts, and analyzes data using advanced scanning technologies

2.	Recording and storage of medical data	▪ Collects, stores, and analyzes medical data to enable faster access and informed decision-making. ▪ Patient information is electronically stored, streamlining diagnosis and treatment. ▪ Tracks and provides daily updates on a patient's progress. ▪ Digitally stored data aids in identifying disease causes and supports research and development. ▪ Maintains a comprehensive medical history of each patient and compares it with illness databases for better insights.
3.	Use of Robots	▪ Aethon TUG robots autonomously navigate hospitals to transport supplies, meals, medications, specimens, and heavy items such as trash and linens. ▪ Available in two configurations: an exchange base platform for moving racks, bins, and carts, as well as fixed and secured cart options.
4.	Training	▪ Lack of medical specialists and facilities leads to high patient mortality in many diseases. ▪ Many patients lose their lives during training by inexperienced doctors. ▪ Untrained medical professionals pose a significant risk of disease complications and fatalities.

4. Conclusion

Machine learning (ML) approaches in drug discovery offer potential to reduce time, costs, and improve safety compared to traditional methods.The introduction of AI driven web browsers like ChatGPT sparked interest in using Transformer models to accelerate drug discovery stages.ML-based models face challenges like generating false positives/negatives, which can lead to incorrect predictions and resource waste. Ongoing in vitro, in vivo, and clinical trials are necessary to validate ML-based drug discovery. Future research should aim to improve data quality, enhance ML algorithm interpretability, and integrate human expertise to increase drug discovery efficacy.

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