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Aim: Intelligence Artificial Intelligence For Drug Discovery In The Context Of Revolutionizing Drug Delivery

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Abstract: Artificial intelligence (AI) is changing drug discovery by speeding up research, lowering costs, and improving success rates. Using methods like machine learning, deep learning, and NLP, AI quickly analyzes large datasets to find drug targets, predict how drugs will work, and improve drug design. It also helps identify side effects earlier and makes clinical trials more efficient through better patient selection and data analysis.Although AI offers many benefits, such as higher accuracy and reduced risks, challenges like data quality, model transparency, and regulatory issues remain. Improving data standards and collaboration will be important for future progress. Overall, AI has strong potential to create safer, more effective, and more affordable medicines.

Keyword: Artificial intelligence, drug discovery, machine learning, deep learning, drug formulation drug, drug design.

Introduction: AI is when machines show human-like intelligence. It is a field that creates methods and tools to copy and improve human thinking. **[1] Drug** discovery aims to find new medicines for diseases, but the traditional process is slow, costly, and often inefficient. On average, developing a new drug takes about 15 years and billions of dollars. Because of these challenges, better and faster methods are needed. Advances in computing and the availability of large datasets have made artificial intelligence (AI) a powerful tool. AI, especially in biological data analysis, is now widely used in the pharmaceutical industry to improve and speed up drug discovery**. [2]** Traditional drug delivery systems have been designed to provide medicines safely and effectively. These include oral or transdermal systems, injections, inhalation products, bio-adhesive systems, nanoscale carriers, and controlled-release forms. Although many of these systems are successful, they have limitations, especially for delivering proteins and nucleic acids. Proteins have complex structures and must be given directly because the body cannot produce them after administration. Their activity can be reduced by factors like enzymatic breakdown, aggregation, or loss of structure.**[3]** AI is improving drug delivery by designing smart nanoparticles that release medicines only when triggered by conditions like pH changes or enzymes. This targeted system reduces side effects and ensures accurate delivery. AI also helps create controlled-release systems that maintain steady drug levels in the body, increasing effectiveness and reducing how often patients need to take their medication **[4].**

History of drug delivery technologies: Before 1950, medicines released the drug immediately. In 1952, Smith Klein Beecham created the first sustained-release system (Spansule), which allowed the drug to be released slowly and work for 12 hours**. [5]**

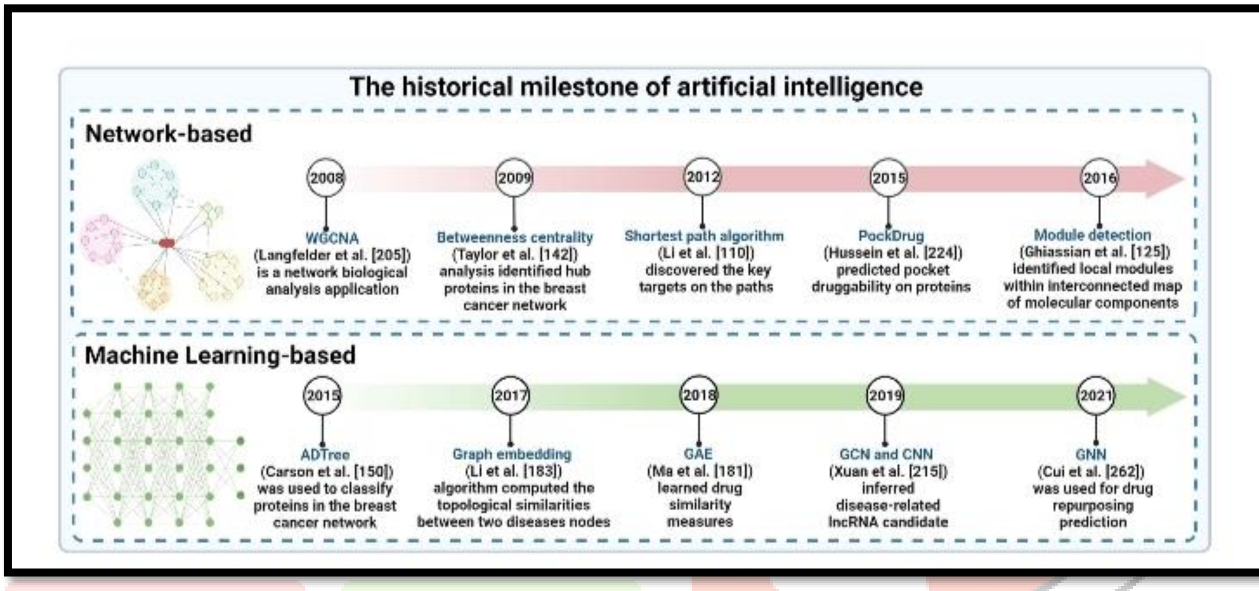

Figure No. 1: The historical milestones of network-based and ML-based biology.

Objectives:

1. **Faster and cheaper drug Discovery:** AI speed up drug development by automating tasks, reducing time and cost.
2. **Better prediction of safety and effectiveness:** AI helps predict how a drug works and its side effects, reducing failure in later stages.
3. **Personalized medicine:** AI analyses patient data to give the right drug and correct dose for each person.
4. **Finding new drug targets:** AI scans large biological data to discover new diseases Targets and useful molecules.
5. **Improved drug delivery systems:** AI designs better drug delivery methods to increase treatment effectiveness and patient adherence.
6. **More efficient clinical trials:** AI helps select patients, predict outcomes, and analyse data to make trials faster and more successful.

Evolution of AI in Drug Discovery:

AI's role in drug discovery began in the 1960s with DENDRAL. Since then, it has expanded to tasks like target identification, lead optimization, and drug design. Early uses focused on predicting compound properties, but modern AI can model protein structures and design targeted drugs, as seen with tools like MolAICal. **[6]**

Basic Principle

Artificial intelligence includes many algorithms and methods. This section briefly outlines the fundamental AI concepts commonly used in drug discovery. Readers who want more background can explore detailed studies, while those already familiar with the basics may proceed to section 2.2 for more advanced topics. **[7]**

Overview AI drug discovery:

The pharmaceutical industry faces growing pressure due to rising research costs and slower progress in traditional drug development. Drug discovery usually takes many years and begins with selecting a disease and identifying a biological target linked to it .Researchers then screen large number of chemical compound to find those that may Interact with the target. These initial promising molecules are known as ―hit‖ compound, and further testing helps determine a stronger, more precise candidate called the lead compound. **[8]**

De novo Drug Design

AI has transformed de novo drug design by enabling the generation of entirely new molecular structures instead of relying on existing chemical libraries. **[9]** Deep learning plays a critical role in computer aided drug design (CADD) because these models can process vast datasets and execute highly complex computations required for modern drug discovery. **[10]**

Drug formulation

AI models like SVM and ANN were used to study how drying conditions—such as starting mass, temperature, water content, and pressure—affect drying time. These models showed very high accuracy, with an R^2 of 0.999 and a very low error (RMSE < 8.8×10^{-3}). **[11]**

AI drug formulation

AI is increasingly used in drug formulation to improve solubility, stability, bioavailability, and overall product performance. By analyzing complex datasets, AI can predict formulation behavior and optimize excipient selection and processing conditions. Quality by Design (QbD) by enhancing precision and manufacturing efficiency. **[12]**

Personalized Medicine and Artificial Intelligence

Medicine is shifting from treating diseases after they appear to preventing them and promoting long-term health. This shift aligns with the concept of P4 Medicine— preventive, participatory, predictive, and personalized care. AI and machine learning. Play a key role in this transition by analyzing large genomic and clinical datasets to predict treatment responses. These technologies support more accurate diagnoses, guide therapy selection, and help clinicians tailor treatments that are both effective and safer for each patient. **[13]**

AI for Predicting Physicochemical Stability

AI uses machine learning and computational models to analyze formulation data and predict the

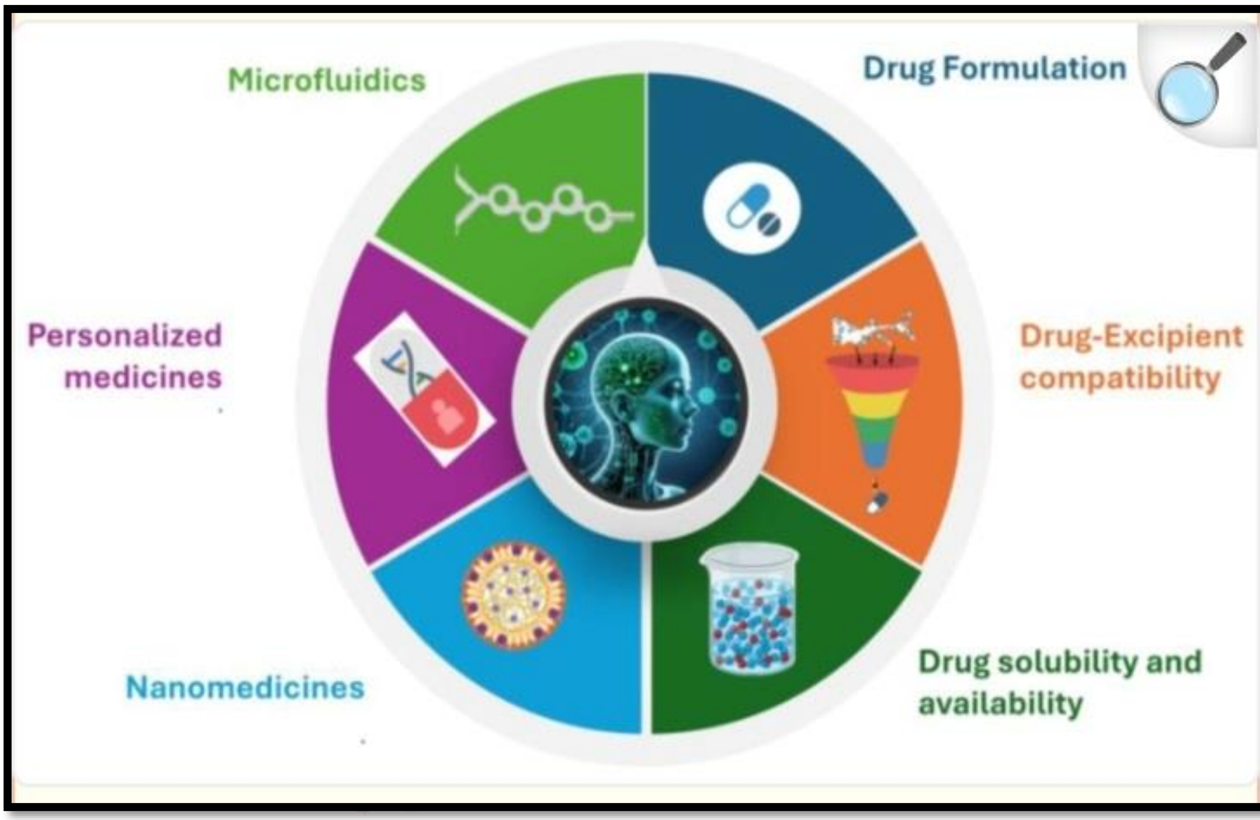

Figure No. 2: AI predictive modeling in personalized medicines, drug formulation, drug–excipient compatibility, drug solubility, bioavailability, nanomedicines, and microfluidics in system.

physicochemical stability of oral dosage forms. By assessing factors such as degradation pathways, ingredient interactions, and environmental influences, AI helps identify potential stability issues early. These insights guide formulation improvements and support decisions that enhance product durability and shelf life. **[14]**

AI in precision medicine and early clinical development

AI can analyze large genomic, proteomic, and clinical datasets to identify biomarkers that predict disease progression or treatment response. By interpreting a patient's genetic profile, AI helps forecast how well they may respond to specific therapies. This enables more personalized treatment strategies and supports the advancement of precision medicine in early clinical development. **[9]**

AI in Nanomedicine

AI enhances nanomedicine by improving data analysis, pattern detection, and system optimization, helping researchers design more precise nanoscale technologies. It supports the development of targeted drug-delivery systems, advanced diagnostics, and personalized treatments. AI models also assist in designing nanoparticles by predicting their behavior, stability, and therapeutic performance, leading to safer and more effective nanomedicine applications. **[14]**

8. Overview of Solid Dosage Formulations Designed by AI

Solid dosage forms such as tablets, powders, and granules remain the most common drug delivery systems due to their convenience, stability, and patient compliance. Their dominance in the pharmaceutical market is expected to continue.AI applications in solid dosage formulation have grown rapidly since research began in the 1990s, with publication rates rising sharply after 2015. Tablet formulations account for over 60% of AI-focused studies, reflecting their central role in dosage design. Recent research highlights the use of AI for formulation optimization, process control, and predictive modelling of critical quality attributes (CQAs). Table 4 provides a summary of key AI applications, illustrating current trends and advancements in solid dosage form development. **[15]**

Tablets

Ma et al. used Convolutional Neural Networks (CNNs) to detect internal defects in tablets. Tablet batches containing mannitol and microcrystalline cellulose were imaged using X-ray Computed Tomography (XRCT), and image augmentation expanded the dataset from 573 to 43,548 images The CNN included three modules: UNet A for separating tablets from the bottle, Module 2 for identifying individual tablets, and UNet B for detecting internal cracks. The system achieved up to 94% accuracy across seven tablet batches. This approach offers a fast and efficient method for identifying defects and may be applied to other manufactured products. **[16]**

Granules

Zhao et al. used AI methods to assess and predict drug concentrations in sugar-free granules. Near-infrared (NIR) spectroscopy enabled accurate measurement of drug content, and machine-learning models—including evolutionary algorithms, PSO/SVM, and backpropagation ANN—effectively predicted residual drug levels. Their results showed that AI is a reliable tool for quantifying drug content in granules. **[11]**

Emulsions

ANNs were employed to develop stable oil-in-water emulsions. Lauryl alcohol concentration and time were found unreliable, while droplet size, zeta potential, viscosity, and conductivity were strong predictors. ANN outputs correlated well with experimental data. An ANN model also accurately predicted microemulsion containing isoniazid and rifampicin using pseudo-ternary phase-diagram data. **[14]**

Capsules

Zhou et al. used an improved CNN to detect capsule defects such as perforations, concave heads, shriveled or nested capsules, and oil stains. L2 regularization and the Adam optimizer reduced overfitting, with SVM and KNN used as comparators. The model achieved up to 97.56%

Advantages of AI in Drug Discovery

1. AI predicts environmental factors that affect drug stability and improves formulation.
2. AI reduces the time and cost of developing new medicines.
3. AI lowers errors and increases accuracy using smart automated systems.
4. AI helps industries like mining by reducing human error and working in tough environments.
5. AI supports daily tasks like GPS and spelling correction.
6. AI assistants help businesses by reducing the need for human effort.
7. AI helps doctors check drug side effects and health risks more easily.

Disadvantages of AI in Drug Discovery

1. AI lacks human judgment and cannot understand experience or emotions.
2. Humans are more creative than AI.
3. Large use of AI may cause unemployment and reduce human creativity.
4. AI systems are costly and require complex design, maintenance, and frequent updates.**[17]**

Application of AI in drug discovery

Target identification and validation

Machine learning (ML) helps find biological targets for new medicines by studying complex biological data. **[4]**

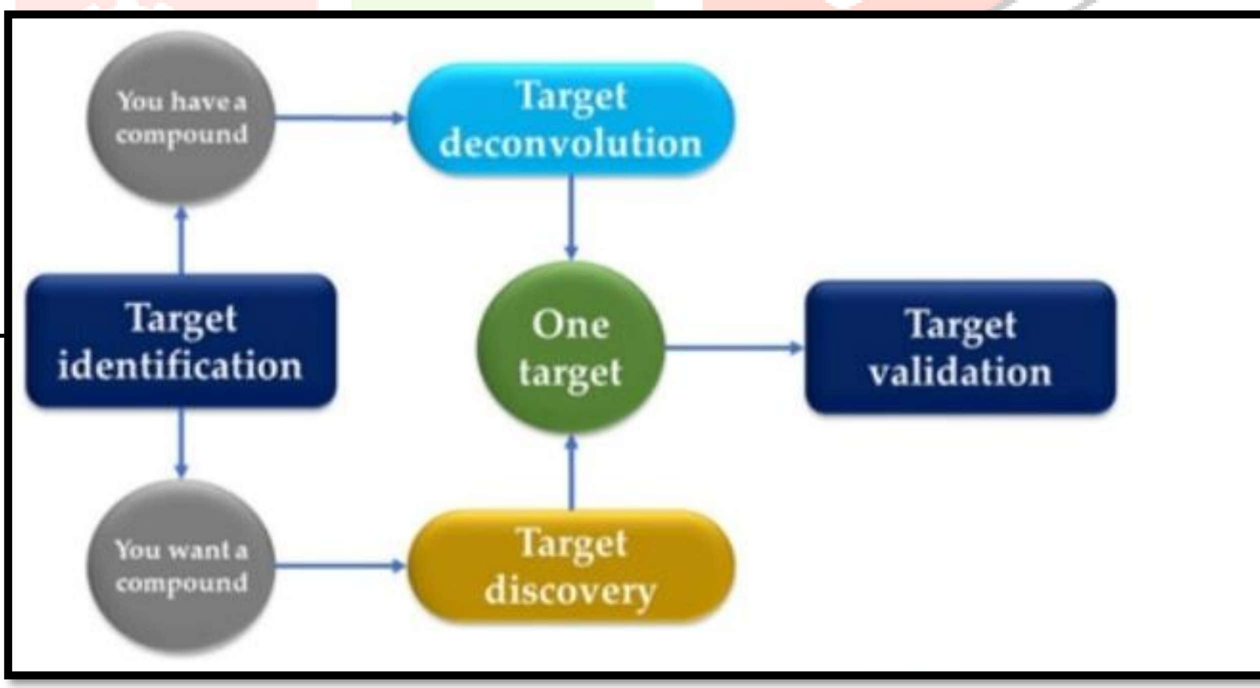

Figure No. 3: Drug development process: target deconvolution vs. targetdiscovery

AI in Drug Screening and lead discovery:

AI helps scientists quickly find which chemical compounds could become useful drugs. Modern algorithms like RF, SVMs, and neural networks can predict toxicity, drug behavior in the body, and how well a compound might bind to a target protein. Earlier drug discovery relied on natural extraction and lab techniques like GC-MS, NMR, and HPLC. With advances in computers, rational drug design became more common Today, AI makes virtual screening faster and more accurate by predicting the best molecules to test. **[18]**

Drug Design and Optimization

Drug design aims to create small molecules that are effective, safe, and chemically suitable, and can be patented. Computer-based tools help a lot in drug discovery, but traditional methods can be slow, expensive, and sometimes unreliable AI can solve these problems and make drug development faster and more efficient. **[19]**

Preclinical and clinical development

AI helps improve drug development by predicting how drugs behave in the body and checking their safety. ML can analyze chemical data to predict absorption, distribution, metabolism, excretion, and toxicity. AI also makes clinical trials faster by improving study design, finding the right patients, and monitoring data in real time. This helps detect safety issues early and supports better treatment decisions. **[20]**

Personalized Medicine and AI

Medicine is moving from treating illness to preventing it, reflected in the P4 Medicine model—preventive, participatory, predictive, and personalized care. AI and machine learning strengthen this shift by analyzing large genomic and clinical datasets to forecast how patients will respond to different treatments. These tools improve diagnosis, guide therapy selection, and support the creation of individualized treatment plans with fewer side effects. **[13]**

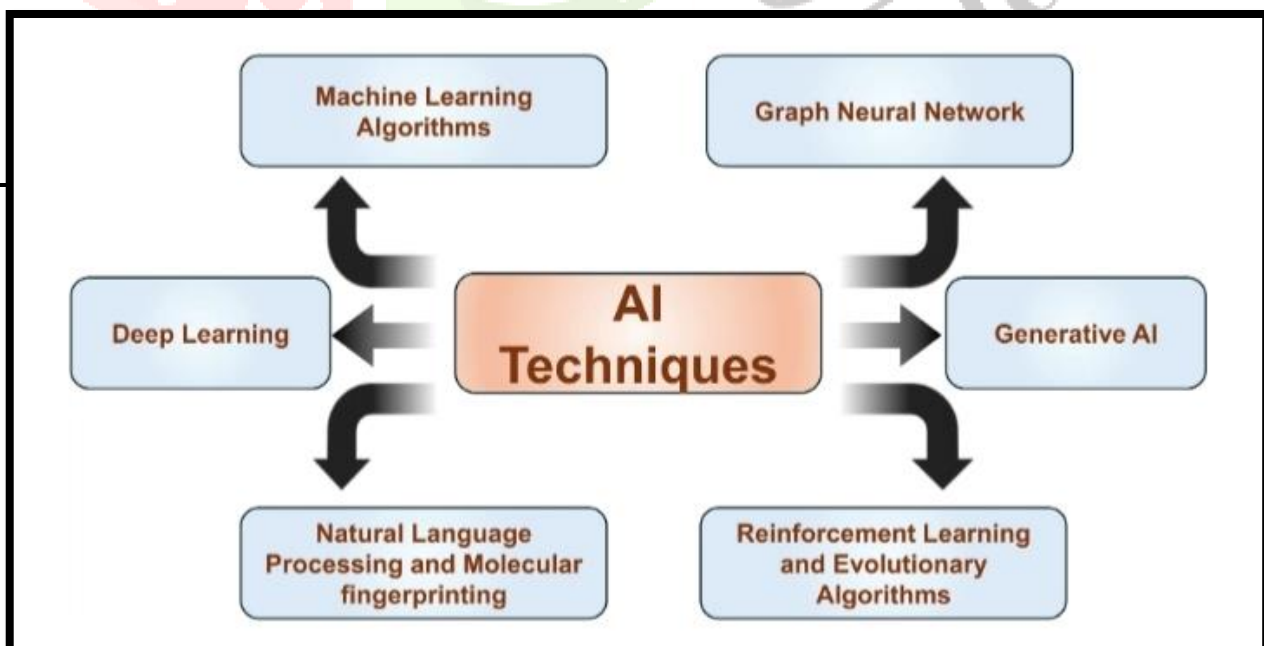

Figure No.4: AI techniques in drugs discovery.

Machine Learning algorithms using supervised and unsupervised learning

Machine learning (ML) is increasingly used in drug discovery and is improving the pharmaceutical industry. Many companies, including large pharmaceutical firms, use ML to support drug research. is important because it can: Speed up drug discovery, reduce costs, decrease workload, and improve accuracy in finding new drugs.**[3]**

Supervised learning: Supervised learning uses labeled datasets to train a model to link input features with known outputs. Because the desired result is defined in advance, the algorithm can learn patterns and make accurate predictions on new data. This approach is widely used in tasks such as image classification, language processing, and predictive analytics. **[21]**

Unsupervised AI Learning: Unsupervised learning analyzes raw, unlabeled data to identify hidden patterns, relationships, and groupings. Without predefined categories, the algorithm discovers structures within the data on its own. This data-driven approach is useful for exploring complex datasets and revealing trends that are not immediately apparent. **[21]**

Deep learning:

Deep learning is a part of AI that processes large and complex data using many layers. It can handle raw it is very useful in medical imaging and bioinformatics to make automatic, reliable, and easy to understand tools. However, it faces challenges like high cost of labelled data, poor quality of biological data, differences in samples, ethical limits in animal studies, and errors due to mismatched medical images. Biological variations also make training harder. Deep learning models must be interpretable, adaptable, reliable, and transparent to overcome these issues. **[3]**

Natural Language processing (NLP):

NLP helps computers understand medical language. It can analyze EHRs, doctors' notes, and test reports to find new information about patients and diseases. This helps create better, personalized care plans. With more digital records available, NLP an improve research and future patient care. **[3]**

Molecular fingerprinting

Molecular fingerprinting turns chemical structures into numeric patterns so computers can quickly compare molecules and use them in machine learning. Common types include ECFP (circular), path-based, and 3D fingerprints. Tools like RDKit and ChemDes help generate these fingerprints for tasks such as virtual screening and toxicity prediction. While useful for finding active compounds and studying structure–activity relationships, fingerprint methods still need improvement to work better across different molecules and biological systems. **[17]**

Reinforcement Machine Learning Reinforcement learning trains a system by allowing it to interact with its environment and learn through trial and error. Instead of being given explicit instructions, the algorithm discovers which actions produce the best results over time. **[13]**

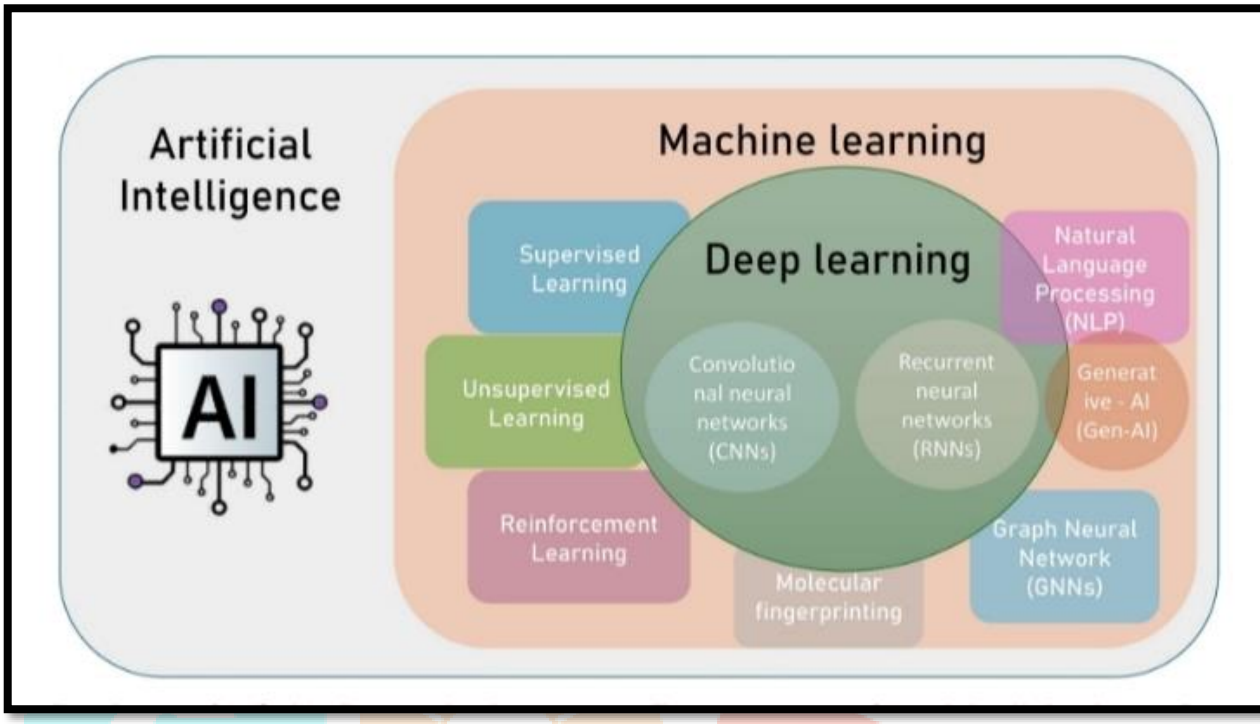

Fig. No. 5: Overview of Artificial Intelligence and its key components. The core components of AI, including Machine learning, Deep Learning, Neural networks, Natural language processing, Molecular fingerprinting, Graph neural network and Generative AI and their Interconnections in AI-driven systems.

Limitations of AI Applied to Early Drug Discovery and Development

AI applications in early drug discovery face several limitations, primarily related to computational constraints, data quality, and ethical or regulatory issues. A major challenge arises from bias in training datasets, particularly when data are not representative of diverse populations. For example, oncology datasets and clinical trials often over represent patients of European ancestry, leading to AI models that perform poorly in underrepresented groups and reducing the accuracy of predictions for patient selection ~~and treatment response .To mitigate these issues, synthetic data (SD) generation is increasingly explored to~~ rebalance datasets and improve model generalizability, though SD may still fail to capture true biological variability .Another limitation involves the reliance on historical or incomplete datasets in drug discovery. Such datasets are often biased toward well-characterized targets or chemical scaffolds, restricting AI's ability to identify novel drug targets or predict properties of innovative compounds. As highlighted by et al. this dependence on outdated or non- standardized data reduces the potential for discovering first-in-class therapeutics. **[9]**Generative AI and QSP Generative AI tools, including LLMs and deep generative models, are reshaping quantitative systems pharmacology (QSP) by creating new hypotheses, automating model building, and supporting the design of novel therapeutics. These models can generate new molecular structures with desired properties, as seen in platforms like Insilico Medicine using GANs and reinforcement learning. Integrating generative AI into QSP streamlines tasks such as data aggregation, parameter estimation, code generation, and report creation. This results in faster, more accurate model development and improves decision-making throughout drug discovery and clinical translation. **[22]**Generative AI Generative AI tools, including systems like ChatGPT, offer significant potential in pharmacy and healthcare by supporting tasks such as prescription review, drug interaction checks, and adverse reaction monitoring. However, their use in pharmacy education and clinical practice is still limited, highlighting the need for further research and implementation studies.Beyond clinical use, generative AI can create large synthetic datasets for training Predictive models. Technologies such as Generative Adversarial Networks (GANs) generate realistic data through a generator–discriminator framework, enabling applications in medical imaging, super-resolution, and data augmentation. For example, Super-Resolution GAN (SRGAN) can enhance low-resolution medical images, demonstrating how generative AI can advance diagnostics and data-driven decision- making in healthcare. **[23]**

Use of multimodal models and QSAR in drug discovery

Multimodal models integrate chemical, biological, and other data types into a unified system, strengthening QSAR analyses. In drug discovery, QSAR methods predict a compound's biological activity from its molecular structure. AI enhances these models by improving pattern recognition and predictive accuracy, enabling faster and more efficient identification of promising drug candidates. **[9]**

Challenge and limitations:

Data quality and availability: High-quality and accessible data are essential for effective AI. AI models need large, well-organized, and diverse datasets to make accurate predictions. However, biomedical data is often messy, incomplete, or inconsistent, which reduces model accuracy and can cause biased results. When certain groups or diseases are underrepresented, AI systems cannot generalize well, limiting their reliability across different populations. **[23]**

Interpretability and transparency: Many AI models function like ―black boxes,‖ making their decisions hard to explain. In pharmaceuticals, this is a major issue because transparency and accountability are required. Explainable AI helps build trust, supports regulation, and ensures responsible decision-making. **[23]**

Ethical challenge of using AL: AI-assisted drug discovery brings ethical and regulatory challenges, including potential algorithmic bias if training data is unrepresentative. Issues like data ownership, data sharing, and the role of AI in patient-care decisions also raise concerns. Addressing these factors is essential for responsible and ethical AI use. While AI can greatly speed up drug discovery and support precision medicine, its challenges must be resolved to fully realize its benefits and improve patient outcomes. **[24]**

AI in real word application AI in drug repurposing:

AI greatly supports drug repurposing by quickly analyzing biomedical literature, clinical data, and molecular profiles to identify new therapeutic uses for existing drugs. It can also uncover effective drug combinations by evaluating complex interactions such as drug–target networks and genomic pathways. These capabilities help reveal promising repositioning opportunities and synergistic therapies that traditional methods may miss. **[25]** AI supports drug repurposing by identifying new therapeutic uses for medicines that are already approved. Instead of developing drugs from scratch, AI analyzes existing safety data, pharmacological profiles, and mechanisms of action to predict whether a drug could work for another disease. This strategy lowers development time and cost while expanding treatment options for conditions that lack effective therapies. **[26]**

Future Directions and Opportunities in AI-Assisted Drug Discovery

The AI-based drug discovery field is expected to grow rapidly. New AI tools such as machine learning, natural language processing, and deep learning help analyze complex biological data and predict how drugs will interact with their targets.AI platforms make virtual screening faster and more accurate, helping researchers find potential drug candidates from large compound libraries. They also assist in optimizing lead compounds and predicting pharmacokinetic and toxicity profiles, which improves the selection of safe and effective molecules. AI is also changing drug design by creating new molecular structures with desired properties. These AI-designed molecules can be customized for specific diseases, offering strong potential for future precision medicine.

Conclusion: AI is reshaping the pharmaceutical field by improving drug discovery, clinical trials, and personalized treatment. By analyzing large datastes, Al can identifiy promising compounds, optimize molecular structures, and predict therapeutic outcome faster and more accurately. It also strengthens clinical research through better patient selection, trial design, and safety monitoring, while supporting personalized care based on genetic data. Machine learning and related technologies accelerate target identification, drug design, trial processes, though challenges remain such as the need for high quality data, model transparency, and ethical guidelines.

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