

# Artificial Intelligence in Pharmaceutical Technology and Drug Delivery System

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**Abstract:** *Artificial Intelligence (AI) refers to advanced computational technologies designed to simulate human intelligence, enabling systems to process information, learn from data, solve problems, and support decision-making. In recent years, AI has emerged as a transformative tool in pharmaceutical sciences, contributing significantly to areas such as drug discovery, formulation development, polypharmacology, and hospital pharmacy operations. In drug discovery, AI techniques—particularly Artificial Neural Networks (ANNs), including Deep Neural Networks (DNNs) and Recurrent Neural Networks (RNNs)—are widely used to analyze complex chemical and biological datasets. These models assist in predicting molecular properties and biological activities through approaches such as quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) modeling. Such predictive capabilities accelerate the identification of promising drug candidates while reducing time and research costs. AI also plays a crucial role in drug delivery and formulation development by optimizing formulation parameters and predicting stability, solubility, and release profiles. Moreover, de novo drug design strategies powered by AI enable the creation of novel molecular structures with desired pharmacological characteristics. Beyond research and development, AI supports hospital pharmacy services through automated dispensing systems, medication error detection, inventory management, and clinical decision support systems. Overall, AI is revolutionizing pharmaceutical practice by improving efficiency, enhancing accuracy, and fostering innovation across multiple domains of pharmacy...*

**Keywords:** Artificial intelligence, Artificial neural network, Drug discovery, Drug delivery research, research, Hospital pharmacy

## I. INTRODUCTION

Artificial Intelligence (AI) is a rapidly advancing branch of science concerned with the development of intelligent computer systems capable of performing tasks that normally require human intelligence. These tasks include learning from experience, reasoning, recognizing patterns, problem-solving, and decision-making. [1] AI systems are designed to simulate aspects of human cognition by collecting data, processing it through structured algorithms, generating conclusions (either precise or predictive), and continuously improving performance through feedback and self-correction mechanisms. [2] In a broader sense, AI incorporates machine learning techniques that enable systems to imitate cognitive processes and adapt without explicit reprogramming. [2,3] AI technology enhances analytical accuracy and provides meaningful interpretation of large and complex datasets. [3] To achieve this, AI integrates statistical modeling, computational intelligence, and advanced algorithmic frameworks. [4] Although rapid technological development has generated concerns regarding employment displacement, most AI innovations are widely welcomed due to their significant contributions to productivity, precision, and industrial growth. In recent years, AI has become a fundamental tool across diverse technical, industrial, and research domains. [3,4] Within pharmaceutical sciences, the adoption of AI has shifted from early skepticism to strong optimism. The integration of AI applications in pharmacy—including drug discovery, formulation development, polypharmacology, and hospital pharmacy practice—has demonstrated substantial potential and practical benefits. [5,6] AI-based systems assist



researchers and healthcare professionals in improving efficiency, reducing development timelines, and minimizing costs. One of the most significant applications of AI in pharmacy is drug discovery. Traditional drug discovery processes are time-consuming, expensive, and often associated with high failure rates. AI-driven models help streamline these processes by analyzing vast chemical and biological datasets to identify potential drug candidates. Artificial Neural Networks (ANNs), particularly advanced architectures such as Deep Neural Networks (DNNs) and Recurrent Neural Networks (RNNs), are widely employed for predictive modeling and data analysis. These models are capable of identifying complex relationships between molecular structure and biological activity. AI techniques are extensively used in quantitative structure–activity relationship (QSAR) and quantitative structure–property relationship (QSPR) studies. These approaches allow prediction of pharmacological activity and physicochemical properties of compounds based on their structural attributes. By leveraging AI, researchers can rapidly screen thousands of compounds and prioritize promising candidates for further experimental validation. The predictive superiority of deep learning models has been demonstrated in competitive scientific challenges such as the Merck Kaggle competition [11] and the NIH Tox21 challenge. [12–14] In these evaluations, DNN-based models often outperformed traditional machine learning algorithms, highlighting their enhanced predictive capability. Another transformative application of AI in pharmaceutical sciences is de novo drug design. AI-powered algorithms can generate entirely new molecular structures with predefined pharmacological or physicochemical properties. [14] By exploring vast chemical spaces computationally, AI systems propose innovative drug candidates optimized for potency, selectivity, safety, and bioavailability. This approach significantly reduces reliance on trial-and-error methods and accelerates early-stage drug development. AI also plays a crucial role in drug delivery and formulation development. Formulation scientists often deal with complex variables such as solubility, stability, dissolution rate, and excipient compatibility. AI models assist in optimizing these parameters by analyzing experimental data and predicting formulation performance. Machine learning systems can forecast in vivo drug responses, pharmacokinetic parameters, and appropriate dosing regimens. [2,7] Accurate pharmacokinetic prediction is particularly important in ensuring therapeutic efficacy and minimizing adverse effects. The use of in silico modeling techniques enhances efficiency and cost-effectiveness in pharmaceutical research. [8] Polypharmacology, which involves the interaction of drugs with multiple biological targets, is another area benefiting from AI integration. Many diseases, particularly chronic and complex disorders, involve multiple pathways and molecular mechanisms. AI tools can analyze network pharmacology data, predict multi-target interactions, and support the development of therapies that address complex disease profiles more effectively. AI technology development can generally be categorized into two major classes. [9] The first includes traditional computational approaches such as expert systems, which are rule-based programs designed to simulate human expertise and reasoning processes. [10] These systems draw conclusions from established principles and structured knowledge databases. The second category consists of neural network-based models that mimic the functioning of the human brain. [9] Artificial Neural Networks, including DNNs and RNNs, are central to this category and represent the driving force behind modern AI advancements. Machine learning, a core component of AI, utilizes statistical methods that enable systems to learn from data either with supervision or independently, without being explicitly programmed for each task. [13] This adaptability makes AI highly valuable in pharmaceutical research, where datasets are often large, multidimensional, and continuously evolving. Beyond research and development, AI significantly contributes to hospital pharmacy and healthcare management. AI-driven systems support automated dispensing, medication error detection, inventory management, and clinical decision support. By analyzing patient data, AI tools can help identify potential drug–drug interactions, optimize dosing strategies, and enhance medication safety. Automation in hospital pharmacy reduces manual workload, minimizes dispensing errors, and improves overall operational efficiency. Despite its numerous advantages, AI implementation requires careful consideration of ethical, regulatory, and technical aspects. Data quality, transparency of algorithms, and validation of predictive models are critical factors in ensuring reliable outcomes. Furthermore, AI is intended to support healthcare professionals rather than replace them. Pharmacists and researchers remain essential for interpreting AI-generated insights and making informed clinical decisions. Overall, AI



has emerged as a transformative force in pharmaceutical sciences. From accelerating drug discovery and enabling de novo molecular design to optimizing formulation development and enhancing hospital pharmacy services, AI offers powerful tools that improve efficiency, accuracy, and innovation. The transition from early enthusiasm to practical implementation reflects growing confidence in the technology.[5,6] As computational methods continue to evolve, AI is expected to play an increasingly central role in shaping the future of pharmacy and healthcare. This review emphasizes the diverse applications of AI in pharmacy, particularly in drug discovery, drug delivery formulation development, polypharmacology, and hospital pharmacy practice. By integrating intelligent computational systems with pharmaceutical expertise, AI has the potential to revolutionize modern healthcare and contribute significantly to patient safety and therapeutic advancement.

#### **ADVANTAGES:-**

Artificial Intelligence (AI) is playing a significant role in advancing pharmaceutical technology and modern drug delivery systems by enhancing productivity, precision, and innovation. One of its primary benefits is the acceleration of drug formulation and product development. Conventional formulation methods rely heavily on repeated experimental trials, which consume considerable time and financial resources. AI-driven tools can evaluate extensive datasets involving excipients, physicochemical characteristics of drugs, stability data, and dissolution behaviour to forecast the most suitable formulation strategies. As a result, development timelines are shortened, research expenses are minimized, and the probability of successful product development increases. In the field of drug delivery, AI supports the design of sustained-release, site-specific, and patient-tailored delivery systems by estimating drug performance within the biological environment. Another significant advantage of AI is its contribution to precision medicine and individualized therapy. By analyzing patient-related factors such as genetic background, age, organ function, and disease state, AI systems can assist in determining optimized dosing regimens and appropriate delivery approaches. This is especially important for advanced delivery platforms including nanoparticles, liposomal carriers, and implantable systems, where precise control of drug release patterns is essential. Furthermore, AI strengthens quality assurance in pharmaceutical manufacturing through real-time monitoring, early detection of production defects, and predictive maintenance of equipment. These capabilities help maintain consistent product quality, support regulatory compliance, and ultimately improve patient safety.

#### **DISADVANTAGES:-**

Despite its many benefits, Artificial Intelligence also presents certain challenges in pharmaceutical technology. A key drawback is the substantial initial investment required for its adoption. Implementing AI-based systems involves the use of sophisticated software, powerful computing infrastructure, trained specialists, and access to extensive, high-quality datasets. For small and medium-sized pharmaceutical companies, allocating resources for such advanced technologies can be financially demanding. Moreover, the reliability of AI outputs is directly linked to the quality and volume of data used for training. If the available data are incomplete, biased, or inaccurate, the resulting predictions may be misleading, potentially causing formulation mistakes or safety concerns in drug delivery applications. In addition, AI introduces regulatory and ethical complexities. Approval from regulatory agencies requires thorough validation, documentation, and transparency of AI-driven processes. However, many AI models operate in a manner that does not clearly explain how decisions are made, often referred to as a lack of interpretability. This limited transparency can create hesitation among regulators and healthcare professionals. Concerns regarding patient data privacy also arise, particularly when personal health information is utilized to design individualized drug delivery strategies. Furthermore, excessive dependence on AI tools may diminish the importance of human judgment, expertise, and critical analysis in pharmaceutical research and development.



**MILESTONES IN AI:-**

Artificial Intelligence (AI) as a term was first introduced in 1956. However, the basic ideas related to AI had already been explored earlier, around 1950, particularly through problem-solving techniques and symbolic reasoning approaches.<sup>5</sup> Several key developments and milestones in the evolution and application of AI are summarized in table 1



Fig.1 Important milestones in the area of AI

**CURRENT PHARMACEUTICAL CHALLENGES AND THE ROLE OF AI**

In the pharmaceutical sector, continuous research is being carried out on small molecules to develop improved therapeutic products and enhance patient satisfaction. Small molecules offer several advantages, including relatively simple chemical synthesis processes and cost-effective preparation of synthetic derivatives. Because of these benefits, many stable and potent formulations based on small molecules are widely used in the pharmaceutical market. However, except in the case of treatments for rare diseases, many newly developed small-molecule drugs face strong competition from generic medicines. Additionally, the launch of innovative small-molecule drugs requires extensive scientific data and multiple stages of clinical trials, which increases financial pressure on pharmaceutical companies and encourages the need for continuous innovation. In contrast, the biomolecular drug industry is expanding rapidly and is helping address some of the challenges associated with small-molecule therapies and the limited dissemination of research innovations. The activity of small molecules mainly depends on their chemical structure and reactivity. Biomolecules, which are comparatively larger in size, typically consist of amino acids forming proteins or nucleotides and ribonucleotides that form nucleic acids. The stability and biological functions of these biomolecules are influenced by their supramolecular arrangements and three-dimensional structural conformations. Several biomolecular drugs, such as Insulin and Adalimumab, have achieved remarkable success in clinical therapy. The pharmacokinetic behaviour of biomolecular drugs is often complex, and administration through infusion is commonly preferred. For nucleic-acid-based therapies, pharmacokinetic modulation



and molecular stabilization are essential research areas. Enhancing pharmacokinetic exposure and improving the stability of these molecular forms remain key objectives in modern drug development. Emerging technological advancements may help overcome many of these challenges and improve therapeutic effectiveness.

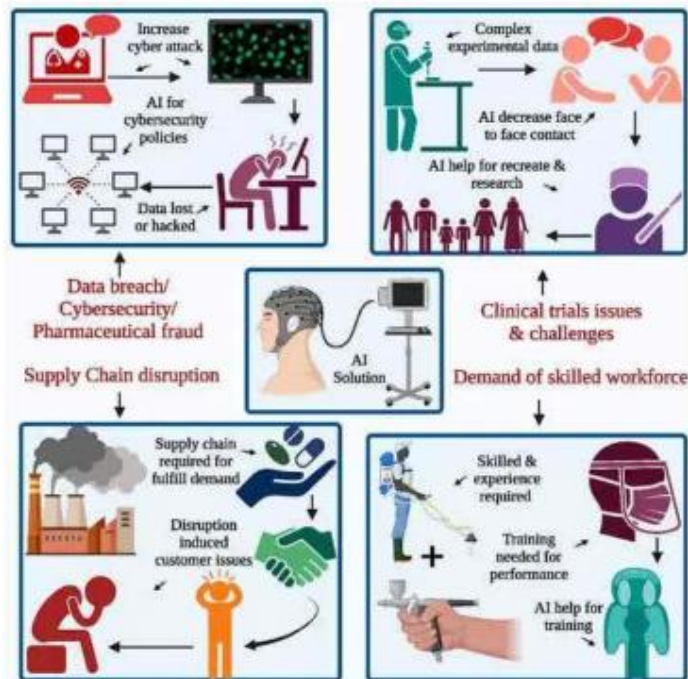


Fig.2 Different supervised and unsupervised AI learning models/tools for pharmaceutical applications

Artificial intelligence (AI) has significant potential in drug discovery and drug delivery research; however, it still has certain limitations that require human expertise for proper interpretation. AI-based predictions are largely dependent on available datasets, and the interpretation of results often involves uncertainty that must be evaluated by researchers. In some cases, algorithmic bias may influence predictions and hypothesis evaluation. Additionally, molecular docking simulations sometimes identify compounds that later prove to be biologically inactive. Therefore, critical evaluation by experts is necessary to verify results and minimize system bias. Despite these limitations, AI offers considerable opportunities for advancing pharmaceutical research. With further development and refinement, AI technologies may reduce current limitations and become more reliable tools in drug discovery. AI methodologies generally rely on machine learning techniques, including deep learning and natural language processing. The learning process may involve supervised or unsupervised approaches, and the selection of appropriate algorithms plays a crucial role in obtaining accurate results. Supervised learning utilizes known input variables (features) and expected outputs (labels or targets) to train predictive models, whereas unsupervised learning focuses on identifying hidden patterns or grouping data with similar characteristics without predefined outputs. In pharmaceutical product development, multiple AI models have been investigated to improve different stages of the development process, and several commonly used models are illustrated in Figure 2.

### AI IN HOSPITAL PHARMACY

Artificial Intelligence (AI) plays an increasingly important role in hospital pharmacy and healthcare systems. It assists healthcare professionals in organizing appropriate dosage forms for individual patients, selecting suitable routes of drug administration, and developing effective treatment strategies. By analyzing large amounts of medical data, AI can improve decision-making and enhance patient care.



### **I. Maintenance of Medical Records:**

Managing patient medical records is often a complex and time-consuming task. AI systems simplify this process by helping in the collection, storage, organization, and retrieval of patient information. Technologies such as the Google DeepMind Health project enable rapid analysis of medical records, allowing healthcare professionals to access important patient data in a short time. This technology has been used in collaboration with Moorfields Eye Hospital NHS Foundation Trust to improve the diagnosis and treatment of eye diseases.

### **II. Designing Treatment Plans:**

AI technology is also useful in developing effective treatment plans for patients. In critical medical situations where selecting the best therapy can be difficult, AI systems analyze previous clinical data, patient reports, and expert medical knowledge to recommend appropriate treatment options. For example, IBM introduced the Watson program to assist oncologists in evaluating cancer treatment strategies by using large datasets and clinical evidence.

### **III. Assistance in Repetitive Medical Tasks:**

AI can support healthcare professionals by performing repetitive tasks such as analyzing diagnostic images and medical reports. Technologies based on deep learning are capable of examining X-rays, radiological scans, echocardiograms, and electrocardiograms to detect abnormalities and diseases. IBM developed an algorithm known as Medical Sieve, which functions as a cognitive assistant with strong analytical and reasoning abilities. Various specialized AI programs are designed to analyze specific body parts and disease conditions, improving the accuracy and speed of medical diagnosis.

### **IV. Health Support and Medication Assistance:**

In recent years, AI technologies have become valuable tools for providing healthcare support and assisting patients with medication management. For instance, Molly, a virtual nurse developed by a healthcare startup, interacts with patients using a friendly voice and visual interface. It helps patients follow treatment instructions and provides guidance for managing chronic conditions between doctor visits. Another example is the AiCure application, which uses a smartphone camera to monitor patients and ensure proper medication adherence.

### **V. AI Support in the Healthcare System:**

AI systems are capable of collecting, analyzing, and comparing large volumes of healthcare data. This information includes patients' medical histories, treatment records, lifestyle habits, and other health-related factors. By evaluating these datasets through advanced algorithms, AI can support healthcare providers in improving disease prevention, diagnosis, and personalized treatment strategies.

## **AI APPROACHES FOR THE DRUGS DISCOVERY**

The drug discovery process generally begins with information obtained from multiple sources, such as high-throughput screening results, fragment-based screening, computational modeling, and previously published scientific data. These sources provide the initial knowledge required to identify potential drug candidates. In this process, the structural characteristics of drug molecules are studied using computer-assisted drug design techniques. After computational analysis, the selected molecules are synthesized through organic chemistry methods. Once the compounds are synthesized or collected, they undergo high-throughput screening (HTS) in primary assays to evaluate their biological activity. Promising candidates are further evaluated through counter-screening and secondary assays to determine important properties such as bioavailability. During this stage, structure-activity relationship (SAR) studies are performed to understand how chemical structure influences biological activity. Drug discovery often involves a continuous cycle of inductive and deductive reasoning, where experimental observations lead to hypotheses, and these hypotheses are tested through further experimentation. This cyclic process helps researchers gradually optimize lead compounds into potential drug candidates. Automation of certain stages in this inductive-deductive cycle can reduce uncertainty and human error, thereby improving the efficiency of drug discovery. Modern pharmaceutical and chemical industries utilize advanced deep learning platforms, such as the NVIDIA DGX-1 system, to analyze vast amounts of scientific data, including patents and genomic information. Since the volume of available biomedical data is too large



for manual analysis, AI-based supercomputing systems are used to process and interpret the data, enabling the identification of relationships between chemical compounds and biological targets. This capability accelerates the discovery of new drug molecules. One of the major areas where AI contributes to drug discovery is the exploration of chemical space, which refers to the enormous number of possible chemical structures that could potentially act as drug molecules. Computational tools allow researchers to explore this chemical space efficiently and identify promising molecular candidates. Machine learning algorithms and predictive models further assist in identifying compounds that are more likely to interact effectively with specific biological targets. Selecting a successful drug candidate from thousands or millions of biologically active compounds remains one of the most challenging steps in the drug discovery process. AI-based methods, such as those developed by BenevolentAI, help researchers narrow down the number of candidate molecules while increasing the probability of identifying effective compounds. In addition, de novo drug design techniques allow scientists to generate entirely new molecular structures through computational methods without relying on previously known compounds. These in-silico approaches use principles of organic chemistry and virtual screening techniques to predict biological activity, toxicity, and other pharmacological properties before laboratory testing. Active learning algorithms also play an important role in discovering novel molecules that may act on specific disease targets. Various in silico approaches, including ligand-based drug design and structure-based drug design, can be applied using available information about molecular targets and structural biology. These techniques use data about small-molecule modulators and biological macromolecules to guide the design of potential drugs. Although AI-generated molecular design is becoming increasingly advanced, some computationally generated compounds may be difficult to synthesize in practice. Therefore, while AI greatly accelerates the identification of promising drug candidates, experimental validation and practical synthesis remain essential steps in the overall drug discovery process.

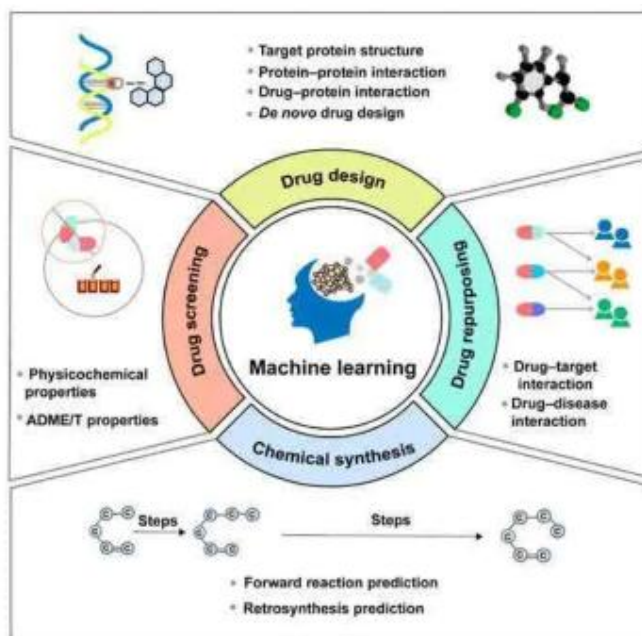


Fig.3 Machine learning empowering drug discovery

Although recurrent neural networks (RNNs) are widely known for their applications in natural language processing (NLP), they have also become valuable tools in the field of de novo drug design. These neural networks are designed to process sequential information, making them suitable for analyzing data that follows a specific order. In drug discovery, molecular structures can be represented using SMILES (Simplified Molecular Input Line Entry System) strings, where chemical structures are encoded as sequences of characters. Because these strings resemble a language format, recurrent neural networks can be trained to understand the “grammar” of SMILES representations. During



training, the networks learn from large datasets of known chemical compounds obtained from databases such as ChEMBL. By studying these datasets, the neural network develops the ability to generate new SMILES strings that correspond to valid chemical structures. One of the advantages of this approach is that recurrent neural networks can generate a large number of chemically valid molecules by processing and producing authentic SMILES sequences. In addition to small molecules, similar strategies have also been applied to design new peptide structures, expanding the potential of AI in pharmaceutical research. Another important technique used alongside neural networks is reinforcement learning, which guides the generated molecules toward desired chemical or biological properties. In this method, the AI system is rewarded when the generated molecules meet specific criteria, such as improved biological activity or favorable pharmacological characteristics. This feedback mechanism gradually improves the quality of the generated compounds. Transfer learning is another useful strategy for generating new molecules with specific biological properties. This approach typically involves two stages. In the first stage, the neural network is trained on a large dataset to learn the basic rules and grammar of SMILES representations. In the second stage, the model undergoes additional training using a smaller set of compounds that possess the desired biological activity. Even a few additional training cycles can guide the model to generate new compounds within a chemical space that is similar to known active molecules. Using these AI-based approaches, researchers have successfully designed and synthesized several novel compounds. In one study, five new molecules were synthesized based on AI-generated designs, and four of these compounds showed activity against nuclear hormone receptors, demonstrating the practical potential of AI-assisted drug discovery.

#### **AI APPROACHES FOR DEVELOPMENT OF DRUG DELIVERY SYSTEMS:-**

The design of drug delivery systems often involves several challenges, such as predicting the relationship between formulation variables and their resulting responses. These uncertainties can influence therapeutic effectiveness and may lead to unexpected outcomes during treatment. When developing advanced or intelligent drug delivery systems, several critical factors must be considered, including controlled drug release, dose adjustment based on patient needs, targeted delivery to specific sites in the body, and the stability of the drug within the formulation. AI-based approaches provide useful tools for addressing these challenges. In particular, algorithms can be applied in self-regulating drug delivery systems to control both the amount of drug released and the timing of release. By analyzing formulation data and performance parameters, AI models can help predict the efficiency of drug dosing and evaluate the drug delivery potential of different dosage forms.

#### **Solid Dispersions**

Artificial neural networks (ANNs), combined with experimental design methods, have been used in the development of solid dispersion formulations. For example, ANN modeling has been applied to create solid dispersions of carbamazepine using carriers such as Poloxamer 188 and Soluplus®. The primary objective of these formulations is to enhance the solubility and dissolution rate of carbamazepine, which is poorly soluble in water. These solid dispersions were prepared using the solvent casting technique. In related research, a feed-forward backpropagation ANN model with a logistic sigmoid activation function was used to analyze the relationship between formulation variables and drug dissolution characteristics. This modeling approach helped identify optimal formulation conditions that improved the dissolution rate of the drug. In another study, mixtures of polyvinylpyrrolidone (PVP) and polyethylene glycol (PEG) were used as carrier materials to prepare solid dispersions. The ANN-based modeling system successfully predicted the formulation parameters required to produce solid dispersions with improved dissolution properties and good physical stability.

#### **Emulsions and Microemulsions**

Artificial neural networks have also been applied in the development and optimization of stable oil-in-water emulsions. In such studies, ANN models are used to evaluate how formulation variables influence the final characteristics of the emulsion. For example, research has been conducted to optimize the concentration of fatty alcohol used in oil-in-water emulsions. Independent variables examined in the model included the concentration of lauryl alcohol and processing



time, while the dependent variables included properties such as droplet size, zeta potential, and viscosity of the emulsion system. By analyzing these relationships, ANN models help researchers design formulations with improved stability and desired physicochemical properties. Overall, AI-based techniques provide valuable support in the formulation and optimization of drug delivery systems by enabling accurate prediction of formulation behaviour, reducing experimental workload, and improving the efficiency of pharmaceutical development.

#### **AI TOOLS APPLICATION IN DOSAGE FORM DESIGNS:-**

The human body is often divided into multiple compartments to better understand how drugs are delivered and distributed. These compartments are simplified representations based on biological membranes that act as barriers within the body. Physicochemical barriers play an important role in determining how drugs move between these compartments, and their influence varies depending on the route of drug administration. One of the key factors affecting the performance of a drug delivery system is the rate of drug permeation through biological membranes. For orally administered drugs, once the medication enters the stomach, it must pass through the gastric or intestinal epithelium before it can reach the bloodstream. This permeation step is essential because it allows the drug to be distributed throughout the body. After entering systemic circulation, the drug travels to its intended target site, which may be a specific tissue, organ, or even intracellular components within cells. In some cases, intracellular molecules themselves serve as the primary targets of drug action. Drug permeation across biological membranes occurs mainly through passive or active transport mechanisms. Passive diffusion is influenced by the physicochemical properties of the drug molecule, such as its size, polarity, and solubility. Computational or in silico models are commonly used to estimate drug distribution and predict permeation behaviour. However, the results generated from these models may differ from actual biological conditions because drug behaviour in the body is also affected by interactions with biological components and the surrounding physiological environment. For certain biologically active compounds and small molecules, passive diffusion is not sufficient for effective absorption or distribution. In such cases, specialized drug delivery systems are required to improve drug transport across biological barriers. Active transport mechanisms involve membrane proteins and complex biological interactions that regulate the movement of drugs into cells or tissues. Because of the complexity of these processes, advanced computational techniques and systematic modeling approaches are needed to accurately study them. Modern computational models are increasingly used to analyze pharmacokinetic parameters related to drug delivery systems. However, one of the major challenges in pharmaceutical research and development is the limited predictability of preclinical models. Predictions are often based on selected parameters, and similar limitations can also occur in complex in silico simulations. Since drug–membrane interactions play a crucial role in drug distribution and absorption, modeling these interactions in simulated environments can provide better insights into drug behaviour. Artificial intelligence offers powerful tools for analyzing such complex and multilayered datasets. AI technologies enable detailed analysis of large amounts of biological and pharmaceutical data, which helps researchers gain deeper insights during drug development. AI-driven models use processes such as simulation, scoring, and refinement to evaluate different parameters during each stage of research. These automated systems can improve prediction accuracy and continuously refine experimental data to enhance the reliability of outcomes.

For effective AI training in biological systems, it is essential to understand drug–biological interactions, which can be studied using system biology databases. AI-based technologies such as artificial neural networks (ANNs) are widely used in pharmacokinetic studies to analyze drug absorption, distribution, metabolism, and elimination. In addition, AI integrates information from various databases, including chemical, genomic, and phenotypic databases, allowing researchers to better understand molecular interactions and the complex biological roles of drugs. AI techniques are also used to evaluate how different drug delivery systems influence the pharmacokinetics and toxicity of pharmaceutical compounds. By analyzing these relationships, researchers can improve the design of dosage forms and optimize therapeutic outcomes. Recent approaches in drug delivery development emphasize identifying critical quality attributes (CQAs) and critical formulation parameters before conducting laboratory experiments. Studying these parameters



through AI-assisted modeling helps predict formulation performance and reduces the need for extensive experimental trials. Overall, the integration of AI in dosage form design provides a systematic and data-driven approach that enhances the understanding of drug–biological interactions, improves predictive accuracy, and supports the development of more efficient and reliable drug delivery systems.

Artificial Intelligence offers several advantages in pharmaceutical research by integrating and analyzing data from multiple sources. It helps researchers identify suitable drug delivery systems that are more likely to produce the expected therapeutic outcomes. AI systems can evaluate complex datasets that include molecular information, patient-specific data, and pharmacokinetic parameters, allowing researchers to determine the most appropriate active pharmaceutical ingredient for treating a particular disease or patient condition. In many cases, passive AI models are used to compare the structural and functional features of new molecular entities with those of previously known compounds. This comparison helps in identifying promising drug candidates and selecting the most suitable drug delivery strategy. Since the effectiveness of treatment often depends on choosing the correct drug delivery system, AI-based analysis improves decision-making and increases the likelihood of achieving better therapeutic results.

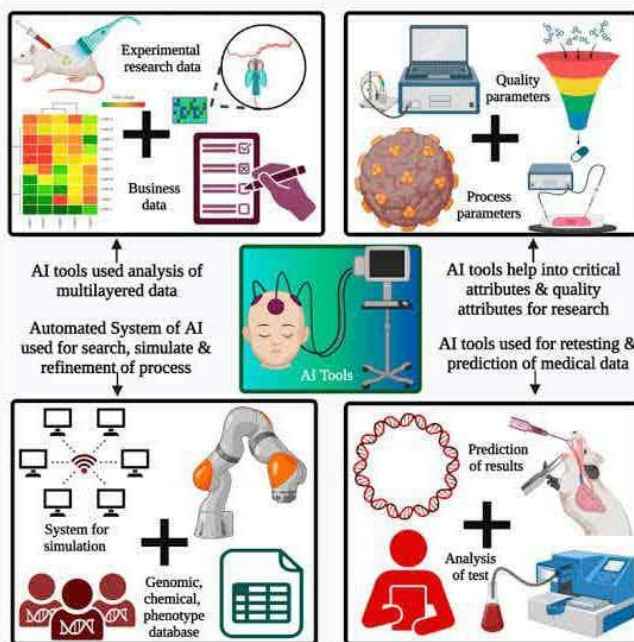


Fig.4 Application of AI Tools in the Pharma Sector

AI also plays an important role in drug discovery and drug repurposing. Drug repurposing involves finding new therapeutic uses for existing medications. By analyzing large datasets related to diseases, molecular targets, and previously approved drugs, AI can identify new treatment possibilities more efficiently than traditional methods. Patient-specific factors and disease characteristics also influence formulation design, pharmacokinetic behavior, and the overall drug development process. Despite its advantages, one of the major challenges in applying AI comprehensively in drug delivery research is the limited availability of well-structured and detailed databases. Reliable datasets are essential for training AI models and ensuring that predictions are accurate and unbiased. Proper evaluation of models and parameters depends heavily on the quality and completeness of the available data. AI technologies support future pharmaceutical innovations by utilizing existing knowledge and continuously learning from new data. These tools can process and interpret large volumes of information, enabling researchers to develop more rational and efficient product designs. Improved knowledge databases, supported by well-documented experimental results and systematic parameter recording, further enhance the performance of AI-driven research models. AI tools are widely used in the



pharmaceutical sector to analyze complex, multilayered datasets. Automated AI systems assist researchers by performing tasks such as data searching, simulation, modeling, and refinement of experimental results during drug development. These capabilities help accelerate research and improve the efficiency of product development processes. Various types of databases are integrated into AI-driven systems to support pharmaceutical research. These include systems biology databases, chemical databases, genomic databases, and phenotypic databases, which provide comprehensive information about molecular interactions and biological mechanisms. In addition, AI-based tools and automated agents can assist in exploring drug models, predicting drug release patterns, evaluating pharmacological activity, and recommending suitable drug delivery strategies. Overall, the integration of AI technologies in the pharmaceutical field enables better data analysis, improves prediction accuracy, and supports the development of more effective and innovative drug delivery systems.

## II. CONCLUSION

Artificial Intelligence is significantly transforming modern drug delivery technologies by supporting the development of targeted, personalized, and adaptive therapeutic systems. Through advanced capabilities in data analysis, pattern identification, and optimization, AI enables pharmaceutical scientists and healthcare professionals to improve drug effectiveness, reduce adverse effects, and enhance overall patient care. AI-driven approaches have also brought major advancements in the study of pharmacokinetics (PK) and pharmacodynamics (PD). Compared with traditional experimental techniques, AI-based models provide several advantages. These systems can estimate pharmacokinetic parameters, simulate how drugs are distributed and eliminated within the body, and assist in determining optimal drug doses and routes of administration. In addition, computational techniques supported by AI can facilitate the development and optimization of physiologically based pharmacokinetic (PBPK) models, helping researchers better understand drug behaviour in biological systems. Such approaches can reduce dependence on extensive animal experiments and large-scale human trials during early stages of research. The emergence of computational pharmaceuticals, supported by artificial intelligence and big data technologies, is reshaping the drug delivery and pharmaceutical development process. This data-driven approach improves the efficiency and cost-effectiveness of drug formulation development while enabling the design of personalized therapies. It also supports regulatory compliance, minimizes development risks, and contributes to improved manufacturing practices. Overall, the integration of AI technologies in pharmaceutical sciences offers strong potential to accelerate drug discovery and development, optimize drug delivery systems, and improve patient outcomes. As these technologies continue to evolve, they are expected to drive the transformation of the pharmaceutical industry from Industry 4.0 toward the more advanced and patient-centered Industry 5.0 era.

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