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REVIEW ON EXPLORING THE ROLE OF ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DESIGN

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ABSTRACT

Artificial intelligence (AI) has emerged as a powerful tool that harnesses anthropomorphic knowledge and provides expedited solutions to complex challenges. Remarkable advancements in AI technology and machine learning present a transformative opportunity in the drug discovery, formulation, and testing of pharmaceutical dosage forms. By utilizing AI algorithms that analyze extensive biological data, including genomics and proteomics, researchers can identify disease associated targets and predict their interactions with potential drug candidates. This enables a more efficient and targeted approach to drug discovery, thereby increasing the likelihood of successful drug approvals. Furthermore, AI can contribute to reducing development costs by optimizing research and development processes. This comprehensive review explores the wide-ranging applications of AI in drug discovery, drug delivery dosage form designs, process optimization, testing, and pharmacokinetics/pharmacodynamics (PK/PD) studies. This review provides an overview of various AI-based approaches utilized in pharmaceutical technology, highlighting their benefits and drawbacks. Nevertheless, the continued investment in and exploration of AI in the pharmaceutical industry offer exciting prospects for enhancing drug development processes and patient care.

KEYWORD:- artificial intelligence (AI); drug discovery; formulation; dosage form testing; pharmacokinetics; pharmacodynamics.

1. INTRODUCTION

"Artificial intelligence in pharmaceutical technology and drug design" is a preference for better stability with high potency to fulfil unmet needs to treat diseases. The assessment of the significant levels of toxicity associated with new drugs is an area of considerable concern, necessitating extensive research and exploration in the foreseeable future. One of the primary aims is to provide drug molecules that offer optimal benefits and suitability for utilization in the healthcare industry. Despite this, the pharmacy industry faces numerous obstacles that necessitate further advancement using technology-driven methods to address worldwide medical and healthcare demands.[5]

Pandemics, natural catastrophes, pricing changes, cyberattacks, logistical delays, and product issues increase supply chain disruptions. Transportation challenges caused by the epidemic have devastated the supply chain network and global industries. Decision induced delays for price updates from suppliers owing to misunderstanding over whether to utilize the new price or the existing price for commodities or materials create price fluctuation delays. New obstacles arise from countries' cross-border trade cooperation strategies, increasing criminal activity and instability in the availability of crucial resources for operation and production. The manufacturing of footprint modifications is needed to suit patient needs and compliance.

Within the pharmaceutical industry, a significant quantity of COVID-19 vaccines ended up being unusable during the pandemic because of complications related to the maintenance of the cold chain. The primary cause of supply chain disruption resulting from the delayed response can be attributed to insufficient innovation and imprecise forecasting in industrial and commercial operations. Supply chain disruptions within the pharmaceutical industry have significant ramifications on customer satisfaction, corporate reputation, and potential profits.[08]

The primary impact of the pandemic is receding, but it still has some influence on clinical trials. Many pharmaceutical companies are looking to adopt newer technologies, including platforms such as AI and virtual platforms in this field. These new technologies may be helpful in the restart or recreation of these clinical trials, with minimal interaction for face-to-face types,[12] as presented in Figure 1. At present, highly skilled workers and high maintenance costs pose a larger challenge. The fourth main challenge in seeking a technology-based solution is data breaches and cybersecurity threats. The number of cyberattacks on available patient data has also increased in the 21st century, and many pharmaceutical companies are more concerned about confidential medical records and patient data, which are especially vulnerable to cybersecurity attacks. Some of the major challenges associated with traditional clinical trials are data fragmentation and disconnected system involvement, which generally result from scattered data generated during the trials and hence require extensive manual data transcription efforts for documents along with those of the systems. There is a lack of innovation in the trial models, which thus requires the rework and repetition of the ongoing work. In the healthcare sector, patient recruitment, enrollment, monitoring, retention, and medical adherence are the key points that require special attention due to clinical trials.[10,11]

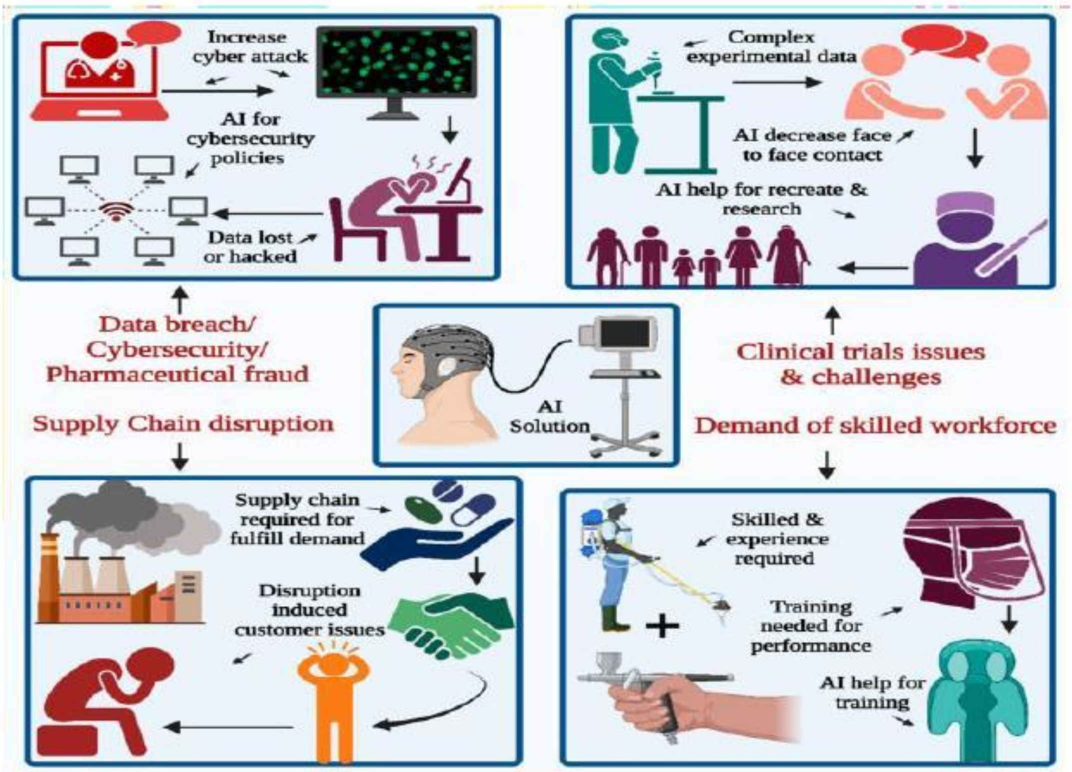

Figure 1: Depicts a possible artificial intelligence (AI) solution to the pharmaceutical industry's challenges: acquiring a proficient workforce is a prerequisite in all sectors to leverage their expertise, proficiency, and aptitude in product innovation. The second pertains to supply chain disruption and clinical trial experimentation challenges. The incidence of cyber attacks is on the rise, with data breaches and security emerging as significant concerns.

2. Current pharmaceutical Challenges and The role of ai

In the pharmaceutical industry, research on small molecules for better products and customer satisfaction is ongoing due to their multiple advantages. The chemical synthesis process is simple, while the synthetic derivative preparation is economical. Thus, many stable and potent small-molecule-loaded formulations are present in the pharmacy sector. Except for the treatment of rare diseases, many innovative small molecules face competition from generic molecules, and complex data are required for them to be launched, along with clinical trials. These processes increase the economic pressure on companies to engage in more innovation. However, the biomolecular drug industry is still growing at a rapid pace to compensate for the crisis induced by the small molecular size and poor dissemination of research and innovations. Small-molecule actions are based on their conformation and reactivity.[20] Biomolecules, which are large units, mostly contain amino acids from the protein source along with nucleotides or ribonucleotides for the nucleic acid. Their stability and function are also influenced by the supramolecular sequence and the spatial conformation.[27] Some biomolecules are very successful products, such as insulin and adalimumab. The pharmacokinetic aspects of these molecules are complex, as infusion is the preferred and most usable route of administration for these biomolecules. Pharmacokinetic modulation and molecular stabilization are important aspects of nucleic acid-based research. The pharmacokinetic exposure and enhancement of these molecular forms are crucial goals. New technological advancement may be helpful to address these challenges and solve related issues.[23] Although there is huge scope for AI in drug delivery innovation and drug discovery, it still presents some major limitations that ultimately require human interference or intellectuals to interpret the complex results.

Regarding AI, the methodology employed involves the utilization of machine learning or its subsets, such as deep learning and natural language processing. The learning process can be either supervised or unsupervised, and the type of algorithm employed is also a crucial factor. Supervised learning is a machine learning methodology that involves the use of known inputs (Features) and outputs (labels or targets), as opposed to unsupervised learning, which deals with unknown outputs.

In pharmaceutical product development, various AI models have been explored to enhance different aspects of the process. A list of commonly explored AI models in this domain is described in Table 1 and Figure 2.

Table 1: Top 5 list of commonly used ai models in the pharmaceutical industry.[1]

AI/ machine learning models	Description/Usage
Generative Adversarial Networks (GANs)	GANs are widely used in drug product development to generate novel chemical structures and optimize their properties.
Recurrent Neural Networks (RNNs)	RNNs are commonly employed for sequence-based tasks in drug development, such as predicting protein structures, analyzing genomic data, and designing peptide sequences.
Convolutional Neural Networks (CNNs)	CNNs are effective in image-based tasks, including analyzing molecular structures and identifying potential drug targets.
Long Short-Term Memory Networks (LSTMs)	LSTMs are a type of RNN that excel in modeling and predicting temporal dependencies. They have been used in pharmacokinetics and pharmacodynamics studies to predict drug concentration-time profiles and evaluate drug efficacy.
Transformer Models	Transformer models, such as the popular BERT (Bidirectional Encoder Representations from Transformers), have been employed in natural language processing tasks in the pharmaceutical domain.

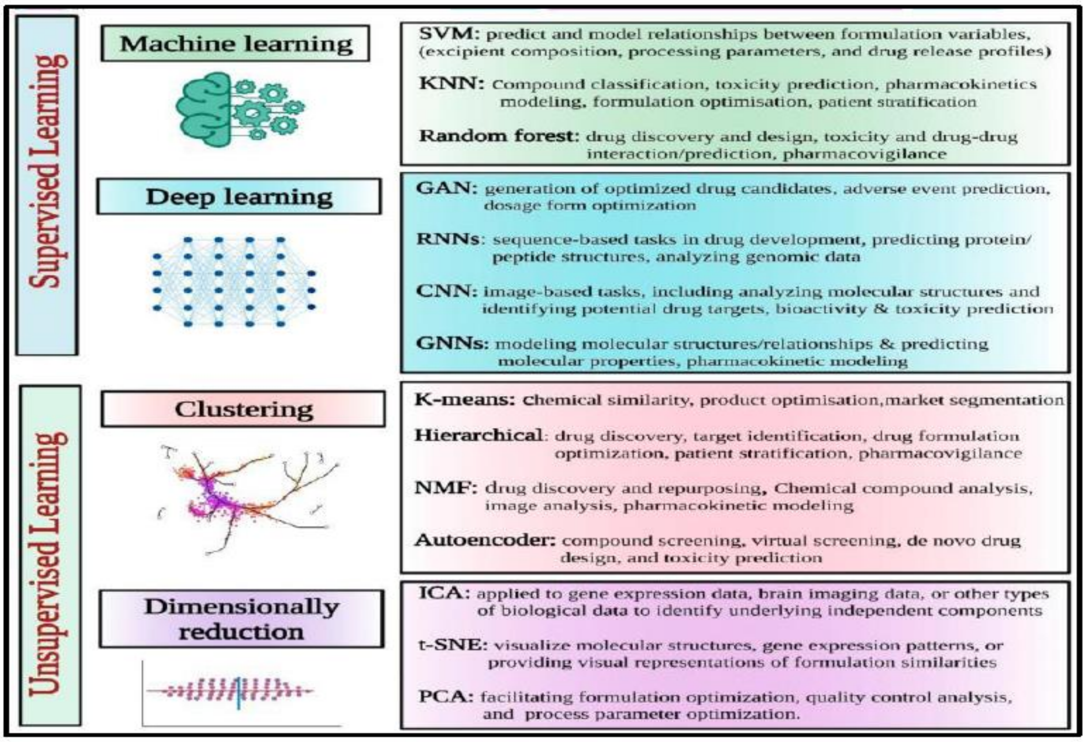

Figure 2: Different Supervised and Unsupervised AI learning models/tools for pharmaceutical applications.[1]

2.1. Supervised AI Learning

Supervised learning refers to a type of machine learning in which an algorithm is trained on a labeled dataset, where the desired output is already known. The algorithm learns to map input data to the correct output by analyzing the patterns and relationships within the labeled data. This approach is commonly used in various applications, such as image recognition, natural language processing, and predictive modeling. Task-driven strategies involve setting specific goals for achieving desired outcomes from a given set of inputs. This approach utilizes labeled data to train algorithms for tasks such as data classification or outcome forecasting. The predominant supervised learning tasks are classification, which involves predicting a label, and regression, which involves predicting a quantity. These techniques include Naïve Bayes, K-nearest neighbors, support vector machines, ensemble learning, random forest, linear regression, support vector regression, and others.[37] It has several applications in the pharmaceutical industry, as described below:

- **Drug Discovery and Design:** Supervised learning algorithms can be used to predict the activity or properties of new drug candidates. By training on a dataset of known compounds and their associated activities, the model can learn patterns and relationships between molecular features and desired outcomes. This enables the prediction of the activity, potency, or toxicity of novel compounds, aiding in drug discovery and design.[38]

- **Predictive Maintenance and Quality Control:** In pharmaceutical manufacturing, supervised learning can be utilized for predictive maintenance and quality control. By training on data from manufacturing processes, equipment sensor data, or quality testing results, the model can learn to predict equipment failure, product quality deviations, or process abnormalities, allowing for proactive maintenance and quality assurance.[39]

- **Drug target identification:** Supervised learning techniques can help identify potential drug targets by analyzing biological data. By training on data that include information about genetic, proteomic, or transcriptomic features and their relationship to drug response or disease progression, the model can learn patterns and identify potential targets for further investigation.[40]

- **Disease Diagnosis and Prognosis:** Supervised learning models can be used to diagnose diseases or predict patient outcomes based on medical data. By training on labeled datasets containing patient characteristics, clinical data, and disease outcomes, the model can learn to classify patients into different disease categories or predict disease progression or treatment response.[42]

- **Adverse event detection:** Supervised learning algorithms can be applied to pharmacovigilance data to identify and classify adverse events associated with drugs. By training on labeled adverse event reports, the model can learn to recognize patterns and identify potential safety signals, helping in the detection and characterization of adverse events.[40]

- **Predictive modeling for clinical trials:** Supervised learning can be used to predict outcomes in clinical trials. By training on historical clinical trial data, including patient characteristics, treatment interventions, and trial outcomes, the model can learn to predict patient response, treatment efficacy, or safety outcomes. This information can guide trial design and optimize patient selection.[40]

2.2. Unsupervised AI Learning

Unsupervised learning refers to a type of machine learning where the algorithm is not provided with labeled data. Instead, it is tasked with identifying patterns and relationships within the data on its own. This approach is often used in exploratory data analysis and can be useful for discovering hidden structures or clusters within a dataset. The approach being described is commonly known as a “data-driven methodology,” which aims to extract patterns, structures, or insights from unannotated data. There are several prevalent unsupervised tasks, including clustering, dimensionality reduction, visualization, finding association rules, and anomaly detection. Various unsupervised learning tasks can be addressed using popular techniques such as clustering algorithms (e.g., hierarchical clustering, K-means, K-medoids, single linkage, complete linkage, BOTS), association learning algorithms, and feature selection and extraction techniques (e.g., Pearson correlation, principal component analysis) based on the data’s characteristics.[45] Unsupervised learning techniques in AI can be valuable for pharmaceutical applications, particularly for exploratory analysis, pattern recognition, and data visualization, as described below:

- **Clustering:** Clustering algorithms group data points based on their similarities, allowing the identification of natural groupings or clusters within the data. In pharmaceutical applications, clustering can be applied to various datasets, such as gene expression profiles, chemical structures, or patient data, to uncover subgroups with similar characteristics. This can aid in target identification, patient stratification, and identifying distinct classes of compounds or diseases.[40]

- **Dimensionality reduction:** Dimensionality reduction techniques, such as principal component analysis (PCA) and t- distributed stochastic neighbor embedding (t-SNE), are used to reduce the complexity of high-dimensional datasets while preserving meaningful information. These methods can help visualize and explore complex datasets, identify key variables or features, and support decision-making processes. Dimensionality reduction can be applied to various types of pharmaceutical data, including gene expression data, drug activity profiles, or imaging data.[43]

- **Anomaly detection:** Anomaly detection algorithms identify rare or unusual data points that deviate significantly from the expected patterns. In the pharmaceutical industry, anomaly detection can be useful for detecting adverse events, identifying potential safety concerns, and uncovering data quality issues. Unsupervised anomaly detection techniques, such as the local outlier factor (LOF) or isolation forest, can help highlight abnormal patterns or data points that warrant further investigation.[40]

- **Association rule mining:** Association rule mining techniques, such as the Apriori algorithm, aim to discover interesting relationships or associations between items in a dataset. In the pharmaceutical context, association rule mining can be applied to drug– drug interactions, adverse event data, or co-occurrence patterns between medical conditions and medications. These techniques can provide insights into potential drug interactions, identify medication patterns, or support pharmacovigilance activities.[48]

- **Topic modeling:** Topic modeling algorithms, such as latent Dirichlet allocation (LDA), extract latent topics or themes from large text datasets. In the pharmaceutical industry, topic modeling can be used to analyze the scientific literature, clinical trial reports, or social media data to identify key research themes, emerging trends, or patient sentiments. This can aid in literature mining, competitive intelligence, or understanding patient perspectives.[41]

3. Ai for drug discovery

AI has revolutionized drug research and discovery in numerous ways. Some of the key contributions of AI in this domain include the following:

3.1. Target identification

AI systems can analyze diverse data types, such as genetic, proteomic, and clinical data, to identify potential therapeutic targets. By uncovering disease-associated targets and molecular pathways, AI assists in the design of medications that can modulate biological processes.

3.2. Virtual screening

AI enables the efficient screening of vast chemical libraries to identify drug candidates that have a high likelihood of binding to a specific target.

3.3. Structure-Activity Relationship (SAR) Modeling

AI models can establish links between the chemical structure of compounds and their biological activity. This allows researchers to optimize drug candidates by designing molecules with desirable features, such as high potency, selectivity, and favorable pharmacokinetic profiles.

3.4. De novo drug design

Using reinforcement learning and generative models, AI algorithms can propose novel drug-like chemical structures. By learning from chemical libraries and experimental data, AI expands the chemical space and aids in the development of innovative drug candidates.

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3.7. Optimization of drug candidates

AI algorithms can analyze and optimize drug candidates by considering various factors, including efficacy, safety, and pharmacokinetics. This helps researchers fine-tune therapeutic molecules to enhance their effectiveness while minimizing potential side effects.

3.8. Drug repurposing

AI techniques can analyze large-scale biomedical data to identify existing drugs that may have therapeutic potential for different diseases. By repurposing approved drugs for new indications, AI accelerates the drug discovery process and reduces costs.

3.9. Toxicity prediction

AI systems can predict drug toxicity by analyzing the chemical structure and characteristics of compounds. Machine learning algorithms trained on toxicology databases can anticipate harmful effects or identify hazardous structural properties. This helps researchers prioritize safer chemicals and mitigate potential adverse responses in clinical trials.

Overall, AI-driven approaches in drug research and development offer the potential to streamline and expedite the identification, optimization, and design of novel therapeutic candidates, ultimately leading to more efficient and effective medications.[31]

The field of drug discovery has seen significant advancements with the use of AI models and tools. Some of the popular AI model tools used for drug discovery are given below. These are just a few examples of the AI model tools available for drug discovery.

3.10. Popular AI model tools used for drug discovery

1) Deep chem
2) RD Kit

3) Chem BERTa
4) Graph Conv
5) Auto Dock Vina
6) SMILES Transformer
7) Schrodinger Suite
8) IBM RXN for chemistry
9) Scape – DB
10) GENTRL (Generative tensorial reinforcement)

4. Ai tool application in dosage form designs

The human body system is divided into several compartments to understand the impact of drug delivery. The compartments are further simplified based on biological membranes. Physicochemical barriers are vital for biological compartments and can be implemented based on the mode of drug delivery inside the body. One of the most significant criteria for efficient drug delivery system monitoring is the rate of permeation based on the route of administration. The orally administered drug, after entering the gastric environment, must permeate through the intestinal or gastric epithelium. This step is vital for the further distribution of the drug into the bloodstream. The distribution step conveys the drug to the target site, which can be tissue or any of the specific cellular components.[30] Intracellular molecules can also act as targets for drug entry into the body. Most of the permeation of drugs is facilitated through biological barriers, either passively or actively. Passive diffusion is based on the drug's molecular features. The Insilco models are used to predict drug distribution through computation analysis, but these results are somewhat different from the actual drug distribution study. The drug's interaction with biological components and the availability of the drug in biological environments have a great impact on the drug's fate in the body. This process is governed by the molecular features of the drug. For many biologically active entities and small molecules, passive permeation is inefficient and requires a specific drug delivery system. The active permeation process is driven by membrane transport and depends on complex biological interactions. This complex process must be explored by using many specific parameters through computation and systematic modeling approaches. The predictability assumption is based on the selected parameters, and the same applies to complex in silico models as well. All these cases are linked to drug interactions with membranes and can be better analyzed by the modeled environment, as presented in Figure 3.

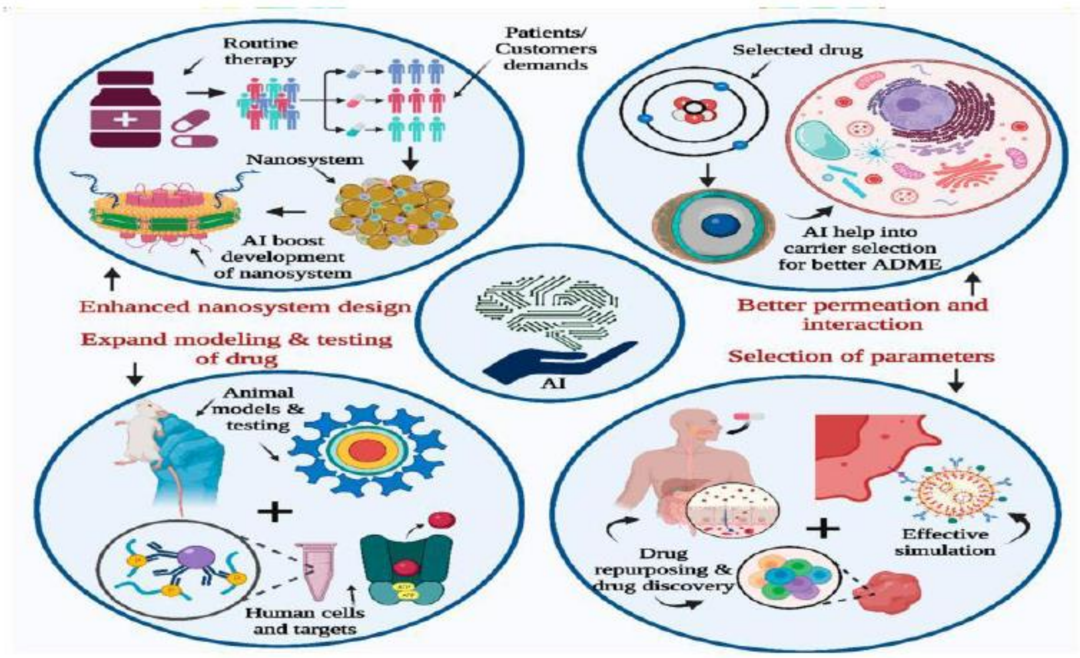


Figure 3: AI contribution to drug development and research.

AI can be used to enhance nanosystem design, expand the present drug testing modeling system, and increase the accuracy of parameter and factor selection in drug design, drug discovery, and drug repurposing methods. It also helps to better understand the mechanism of membrane interaction with the modeled human environment by studying drug permeation, simulation, human cell targets, etc.[1]

The benefits of AI are that it collects information from multiple sources and provides indications for the selected drug delivery system to work as per the anticipated results. The evaluation of the molecular information, patient data, and pharmacokinetic data are considered part of the complex data for analysis for the possible selection of the best active pharmaceutical against patient diseases or requirements. The passive type of AI is implemented for the identification of molecular entity features against those of known molecules for comparison. Effective treatment depends on the accuracy of the selection of drug delivery systems, which are provided by AI.

AI is also useful for the drug discovery process along with the drug repurposing method. This addresses the application of the existing therapeutics to that of the new disease. The requirement of the patients and disease condition are major factors contributing to formulation, pharmacokinetics, and drug development. One of the major challenges associated with the application of AI in full scope to develop delivery systems is the availability of databases with detailed information. This is required for the evaluation of the models, along with parameters, in an unbiased way. AI provides help for future applications by using current knowledge.

5. AI for drug delivery

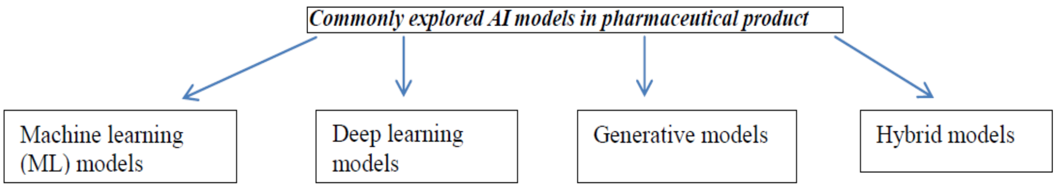
The integration of AI and big data in the field of pharmaceutics has led to the development of computational pharmaceutics, which aims to enhance drug delivery processes by utilizing multiscale modeling approaches. By simulating drug formulation and delivery processes, researchers can evaluate various scenarios and optimize drug delivery systems without the need for extensive trial-and-error experiments. This accelerates the drug development timeline, reduces costs, and increases productivity. Computational pharmaceutics involves modeling drug delivery systems at different scales, ranging from molecular interactions to macroscopic behavior. AI algorithms can analyze complex relationships between drug properties, formulation components, and physiological factors to predict drug behavior at each scale. This allows for a more comprehensive understanding of drug delivery mechanisms and aids in designing efficient drug delivery systems. It helps in the prediction of the physicochemical properties of the drug, the in vitro drug release profile, and the stability of the drug.

5.1. AI for Oral Solid dosage form development

AI involves the use of advanced tools and software to achieve human-like capabilities. Such innovation has helped in many sectors, such as the pharmaceutical industry, especially in the product development phase over the past few years. The implementation of these technological innovations can save time, money, and resources required for manufacturing and proper distribution to end customers through the supply chain. It also provides a better platform to understand the impact of process parameters on the formulation and manufacturing of products.

In the pharmaceutical market, solid dosage forms are predominant, and tablets are one of the dominant dosage forms in this domain. The preparation of the tablet includes many factors based on the type of tablet. AI can help in the search for optimized formulation and the study of the desired attributes involved in the same. AI is also expected to process obligations with the help of automated algorithms and technologies. The implementation of AI also poses a challenge to the regulatory authorities to redefine the policies regarding current good manufacturing practice (cGMP). Different technologies in AI, such as artificial neural networks (ANNs), fuzzy logics, and neural networks, along with genetic algorithms, are implemented for the development of solid dosage forms and a better understanding between the inputs and outputs for processing and operations. ANN is used for better prediction abilities for solid dosage forms, while genetic algorithms are used to predict the results obtained from the utilization of input parameters.[34]

- **List of commonly explored AI models in pharmaceutical product development**



1) Machine learning (ML) models

a) Supervised learning models

- Random forests – used for predicting drug – target interaction and toxicity.
- Support vector machines (SVMs) – applied in molecular property prediction.
- Gradient boosting (e.g., XGBoost, LightGBM) – Helps in clinical trial outcomes prediction.

b) Unsupervised learning models

- K- means clustering – used for patient stratification and biomarker discovery.
- Principal component analysis (PCA) – applied in dimensionality reduction.

c) Reinforcement learning (RL) – models

- Deep Q networks (DQN) – Helps in optimizing molecular design for drug discovery.
  Proximal policy optimization (PPO) – Used in synthetic route optimization for pharma compounds.

2) Deep learning models

a) Neutral networks

- Artificial neural networks (ANNs) – used in drug response prediction and formulation development.
- Convolutional neural networs (CNNs) – applied in image-based drug screening and pathology analysis.
- Recurrent neural networks (RNNs) & Long short – term memory (LSTM) – used in analyzing sequential biological data and clinical trial reports.

b) Transformers
- BERT (BioBERT, ChemBERTa, SciBERT) – helps in processing biomedical literature and extracting relevant insights.
- AlphaFold – developed by DeepMind, used for protein structure prediction.

3) Generative models

a) Variational autoencoders (VAEs) – used in molecular generation and property prediction.
b) Generative adversarial networks (GANs) – applied in de novo drug design and molecular synthesis.
c) Bayesian optimization – helps in optimizing compound properties and drug formulations.

4) Hybrid models

a) Graph neural networks (GNNs) – used for predicting drug- talent interactions and molecular dynamics.
b) Multi – omics models – integrate genomic, proteomic, and metabolomic data for biomarker discovery.

5.1.1. Prediction of dug release through formulations

The prediction of drug release certainly has the potential for stable quality control. Drug release studies are performed through in vivo and in vitro methods, which are treated as fundamental technologies regularly evaluated or tested during product development. The release of the drug from oral solid dosage forms is based on the contribution of critical material attributes along with the processing parameters. Some of the common factors affecting drug release include compaction parameters such as the pressure used for tablet hardness setting, geometric aspects of the tablets, and drug loading characteristics. Many analysis techniques, including spectrophotometric analysis methods, have been implemented, or drug release studies are usually required for extensive analysis.

The drug release results must be set as per the formulator's requirements and require repetitive testing and preparation of the batches to obtain an optimized batch, which makes this task tedious and time-consuming.[10] AI is implemented in the drug formulation and will assist in the prediction of drug release; hence, there is a limited number of runs required to optimize the batch, which further induces a reduction in the work and cost during pilot batch scale and production processes. AI can help predict the drug release profiles and dissolution profiles and explore the disintegration time for the effective selection of the best batch for further scale processing. Some researchers have implemented AI algorithms for the prediction of dissolution profiles into the hydrophilic matrix type of sustained-release tablets with the help of artificial neural networks (ANNs). The support machine vector (SVM), as well as regression analysis, are also implemented during the analysis of the data and prediction of the dissolution profile. The data for the modeling study of drug release were obtained with the help of process analytical technology (PAT) along with critical material attributes. The particle size distribution was found to be the most crucial variable during model prediction. Finally, the ANN was implemented for the identification of the most accurate models as part of the evaluation metrics, as presented in Figure 4.[23]

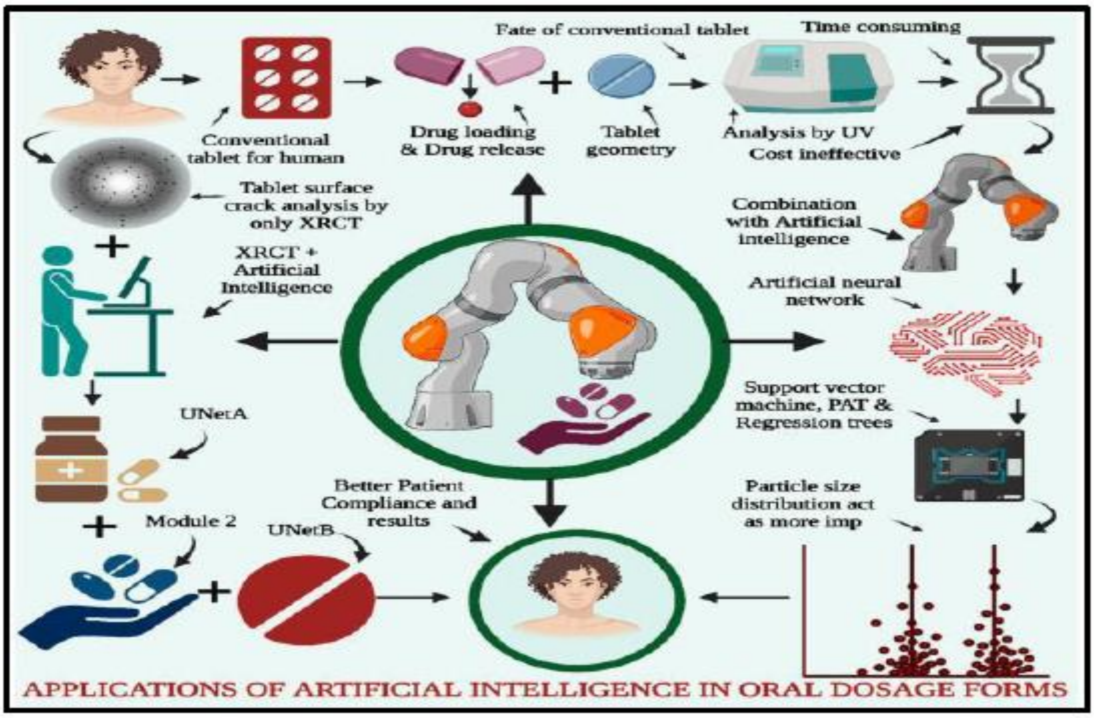


Figure 4: AI for Oral Dosage Forms.

Conventional tablet analysis is performed by screening many factors, such as drug release, drug loading, and study of the tablet geometry and hardness, by using in-process quality control tests along with ultraviolet spectrophotometry. These methods are often time-consuming and cost-ineffective to the industry. To address these issues, the combination of such traditional techniques along with AI was performed by using ANN, SVM, PAT, and regression trees. The data analysis and drug release predictions indicated that particle size distribution was a crucial factor for the same. Defective tablet surface crack analysis is performed by XRCT in combination with AI, containing three modules for distinguishing features for effective application in the healthcare sector.[1]

5.1.2. Application of AI for the Detection of Tablet Defects

The application of AI in the detection of tablet defects has revolutionized quality control processes in pharmaceutical manufacturing. AI algorithms and computer vision techniques are employed to analyze images of tablets, enabling the automated and efficient detection of defects such as cracks, chips, discoloration, or variations in shape and size. By training AI models on large datasets of labeled images, the system learns to accurately classify and identify different types of defects, achieving high levels of precision and recall. Conventional methods, such as X-ray computed tomography, have been used to analyze the internal structure of tablets, but they are still time-consuming and affect the demand for the rapid production of tablets. Deep learning is implemented along with X-ray tomography to detect tablet defects. Ma et al. explored the application of neural networks for tablet defect detection with the help of image analysis completed through X-ray tomography. These researchers have manufactured several batches of tablets by using excipients such as microcrystalline cellulose along with mannitol. The prepared batches were analyzed with the help of the so-called image augmentation strategy. Three different models were used during the same research, including UNetA, which is applicable for the identification of distinguished characteristics of tablets from those of bottles. Module 2 was used for the identification of individual tablets with the help of augmented analysis. The internal cracks in the internal structure of the tablet were analyzed with the help of UNetB. Such UNet networks have been used to check tablet defects with better accuracy and thus provide ease of identification of defects with significant reductions in time, financial costs, and workload. This AI-powered detection not only improves the speed and accuracy of defect identification but also reduces the dependence on manual inspection, minimizing human errors and subjective judgment. The real-time monitoring capabilities of AI systems ensure the prompt detection of defects, facilitating timely intervention and preventing the release of faulty tablets into the market. Ultimately, the integration of AI into tablet defect detection enhances product quality, increases productivity, and ensures the safety and efficacy of pharmaceutical products.

5.2. AI for Nanomedicine

By harnessing AI's capabilities in data analysis, pattern recognition, and optimization, nanomedicine researchers can accelerate the development of novel nanoscale interventions, improve diagnostics, enhance drug delivery, and advance personalized medicine. AI in nanomedicine holds great potential for revolutionizing healthcare by enabling precise and targeted therapeutic approaches at the nanoscale. Nanoparticles are used for targeted drug delivery, imaging, and sensing. AI algorithms can aid in designing and optimizing nanoparticles by predicting their physicochemical properties, stability, and efficacy. This helps researchers develop nanoparticles with desired characteristics for specific applications. Nanomedicines are used effectively as drug delivery carriers for drugs or combinations of drugs based on the concept of drug synergy, especially for the treatment of cancer patients. They contain major impactful inputs, such as drug selection, dose selection, and stimuli-responsive material selection. The deep learning type of algorithm was used for melanoma and has shown great accuracy in caring for patients and assisting in diagnostic procedures.[8]

AI algorithms can model the behavior and interactions of nanoscale materials within biological systems. This enables the prediction of nanoparticle behavior, drug release kinetics, and potential toxicity, facilitating the development of safe and effective nanomedicine formulations. AI can be used in nano sensors and biosensors for the real-time monitoring of biomarkers, drug levels, or disease progression. These sensors can provide continuous feedback to healthcare providers, enabling timely interventions and personalized treatment adjustments.[12]

The AI-based database is useful for scaling up nanocarriers by using an automated system. AI is also used in nanocarrier drug delivery systems, particularly in the optimization of nanocarriers and drug compatibility testing by using computational approaches. Such approaches are used for the evaluation of drug loading, formulation stability, and drug retention. Thus, AI intervention contributes to the enhancement of the therapeutic nanocarriers required for specific cell types for the treatment of tumors. Yuan He et al. studied the application of machine learning methods to the prediction of nanocrystals prepared by high-pressure homogenization along with the wet ball milling method. The demands for a repetition of the experiments can also be decreased by using computational techniques through Monte Carlo simulations and molecular dynamics, along with theoretical techniques. The simulation techniques are helpful for quantitative measurements in critical experiments. AI is also implemented for the creation of the database repository required for nanocarriers, which further helps in the determination of 3D structures along with physical and chemical property investigations in collaboration with structural nanobiology. Such repositories are essential to investigate the relationship between nanocarrier structure and toxicological, physical, and biological data.[17]

5.3. Current trend: Fairy tale to the holy grail

The current trends demonstrate the wide-ranging impact of AI in pharmaceutics, spanning drug discovery, precision medicine, formulation optimization, clinical trials, safety monitoring, and supply chain management. Here are some prominent trends:

- **Drug Discovery and Development:** AI is revolutionizing the drug discovery process by enabling virtual screening, molecular modeling, and predictive analytics. AI algorithms can analyze vast amounts of chemical and biological data to identify potential drug candidates, optimize lead compounds, and predict their properties. This expedites the identification and development of novel therapeutics.

- **Precision medicine:** AI is being utilized to advance precision medicine approaches. By analyzing patient data, including genomics, proteomics, and clinical records, AI algorithms can identify patient subgroups, predict treatment responses, and assist in personalized treatment decision-making. AI also contributes to the development of biomarkers for disease diagnosis and prognosis.

- **Drug repurposing:** AI is being applied to identify new uses for existing drugs, a process known as drug repurposing. By analyzing large datasets and biological knowledge, AI algorithms can identify potential drug–disease associations and repurpose approved drugs for new therapeutic indications. This approach offers a faster and more cost-effective route to drug development.

- **Drug Formulation and Delivery:** AI plays a role in optimizing drug formulations and delivery systems. AI models can predict drug release kinetics and absorption profiles and optimize formulations for enhanced efficacy and targeted delivery. AI is also used to design drug delivery devices and systems that improve patient adherence and convenience.

- **Clinical trial optimization:** AI is being leveraged to optimize clinical trials, improving efficiency and reducing costs. AI algorithms can aid in patient recruitment, identify suitable trial populations, and optimize trial protocols. AI also assists in the real-time monitoring and analysis of trial data, allowing for adaptive trial designs and faster decision-making.

- **Regulatory Compliance and Safety:** AI is increasingly used to support regulatory compliance and ensure drug safety. AI algorithms can analyze real-world data, adverse event reports, and the literature to identify potential safety issues and monitor post marketing drug safety. AI also helps in pharmacovigilance, signal detection, and adverse event prediction.

Table 2: List of companies using Ai and Ml technologies in pharmaceutical research.[1]

Sr. No.	Domain	Technology and Outcome	Industry and collaboration
1.	Drug design	Novel therapeutic antibodies	Exscientia
2.	Molecular drug delivery	Atom Net – deep learning – driven computational platform for structure-based drug design.	Atomwise
3.	Gene mutation related disease	Machine learning based recursion operating system for biological and chemical databases.	Recursion
4.	Drug design	Liga s structure based de – novo drug design	Iktos
5.	Drug target and drug development	Chat panda GPT	Insilico medicine
6.	Drug development	Protein motion in drug development lie RLY – 4008 (Novel allosteric, pan mutant)	Relay therapeutics
7.	Drug research	Automate medical literature review by using natural language processing	Sanofi

6. CONCLUSIONS

AI is transforming drug delivery technologies, enabling targeted, personalized, and adaptive therapies. By leveraging AI's capabilities in data analysis, pattern recognition, and optimization, pharmaceutical researchers and healthcare professionals can enhance drug efficacy, minimize side effects, and improve patient outcomes. AI-based methods have revolutionized the field of pharmacokinetics and pharmacodynamics. They offer several advantages over traditional experimental methods. AI-based models can predict pharmacokinetic parameters, simulate drug distribution and clearance in the body, and optimize drug dosage and administration routes. AI-based computational methods for PBPK models can simplify the development of such models and optimize their parameters, reducing the need for animal studies and human clinical trials. Computational pharmaceutics, facilitated by AI and big data, revolutionizes the drug delivery process by providing a more efficient, cost-effective, and data-driven approach.

It enables the optimization of drug formulations, personalized therapies, regulatory compliance, and risk reduction, ultimately leading to improved drug manufacturing processes and enhanced patient outcomes. Overall, the integration of AI technologies holds great promise for accelerating drug development, improving patient outcomes, and revolutionizing the pharmaceutical industry, promoting its evolution from era 4.0 to era 5.0.

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