

THE GALEN

A PHARMACY MAGAZINE

EIGHTH EDITION: DECEMBER 2025

THEME:

ARTIFICIAL INTELLIGENCE
IN PHARMACEUTICAL TECHNOLOGY
AND **DRUG DELIVERY** DESIGN

PUBLISHED JOINTLY BY:



SAGAR INSTITUTE OF PHARMACY AND TECHNOLOGY
GANDHI NAGAR, BHOPAL

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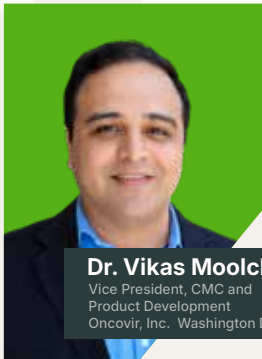
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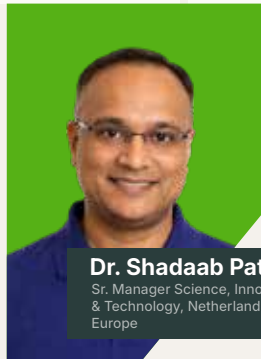


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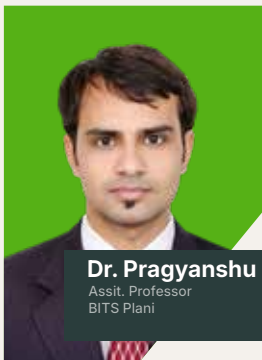
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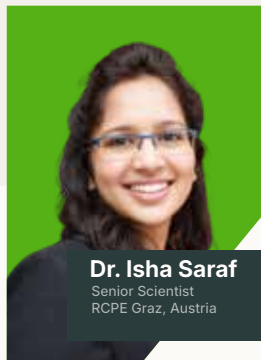
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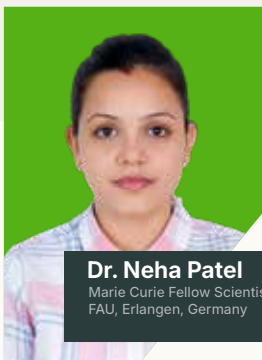
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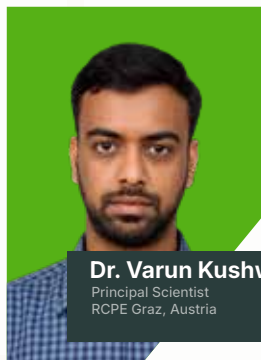
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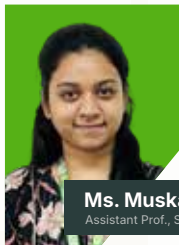
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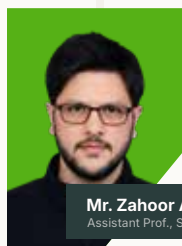
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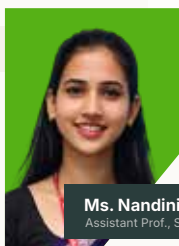
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ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY DESIGN

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INTRODUCTION

"AI" means Artificial Intelligence. It refers to representation of human intelligence process by software, machines enabling them to perform task that typically require human intellect, such as learning, problem solving and decision making.

Today pharmaceutical technology faces several key challenges including regulatory hurdles, talent issue, data security, intellectual property concern and the rising cost and time, research and development also.

KEY CHALLENGES

- Regulatory compliance
- Talent shortage
- Supply chain management
- Data security and intellectual property
- Cost of R&D
- Resistance to change
- Technological interaction
- New drug candidates suffer from poor solubility and efficacy
- Counterfeit pharmaceutical

While AI also significant potential in drug discovery and development, it also present ethical challenges. Ensuring transparency avoiding algorithmic errors and maintaining human oversight are crucial. The pharmaceutical industry is experiencing a significant transformation with the AI. AI is transforming drug discover, development and delivered enabling more efficient and effective option.

BENEFITS OF AI

Increased efficiency: AI can automate tedious task, release up researcher to focus on high value job.

Upgrade accuracy: AI can reduce errors and improve the accuracy of drug development and delivery.

Intensify patient outcome: AI can help personalize treatment plans leading to better patient outcome and improve quality of life.

APPLICATION OF AI IN PHARMACEUTICAL TECHNOLOGY

Drug Discovery: Algorithms of AI can analyze broad amount of data to identify potential drug candidates, predict their efficacy and optimize lead compound. In pharmaceutical industries drug discovery is costly time-consuming process. AI helpful for reducing cost as such enhancing efficacy and increase success rate.

AI algorithms analyze genomic, Proteomic and metabolomic data, biological targets implicated in specific diseases. This helps researchers identify promising targets for drug developments and increase the drug discovery process. AI virtually screen huge data of chemical compound to identify those most likely to interact with a specific target. This reduces time and cost associate with screening.

Personalize medicine and prediction of drug properties: AI models can predict a compound Pharmacokinetic and pharmacodynamic properties such Absorption, Distribution, Metabolism and excretion this help researchers' priorities and promising of drug development. AI can customize treatment plans individual patient based their genetics profile, medicine history and lifestyle and tailor therapies individual patient leading to more effective and personalize treatment

Drug delivery design: AI can be used to design new molecules with desired properties. AI can optimize drug delivery system such as nanoparticles, microparticles to improve solubility, stability and bioavaibility and other characteristics.

Improve clinical trials: Alcan help optimize clinical trial design, monitor trial process, identify suitable patient, potentially reducing the time and cost of clinical trials.

CHALLENGES OF AI

AI in Pharmaceutical industry faces challenges including data quality, modal interpretability, integration with existing work flow and ethical consideration. AI modal especially deep learning requires high quality data base for training and validation. That comesfrom diverse sources making it challenging to integrate and standardize. A big hurdle is ensuring access to relevant data, especially in standardized format protecting sensitive patient data and preventing data branches are crucial aspects AI based drug discovery.AI in pharmaceutical technology raises ethical concern about data privacy algorithmic bias and potential for misuses. A clear guideline for validation, transparency and ethical use not available today a proper regulatory framework is needed. A shortage of professional with AI tools are necessary to established drug development, new technology.

CONCLUSION

AI is changing the pharmaceutical industry by improving drug discovery, personalized medicines and drug delivery design while challenges and limitation exist. The benefits of AI in pharmaceutical technology are significant and its adaptation is expected to continue growing the future.

ARTIFICIAL INTELLIGENCE (AI): A BOON IN PHARMACEUTICAL SECTOR

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INTRODUCTION

Throughout the world a large number of industries are striving to boost their progress towards increasing demands and expectations of their customers, thereby utilizing various methodologies. As per the reports of World Counts approximately 60 million people die worldwide each year being roughly equivalent to the population of South Africa. Meanwhile the World Health Organization provides the fact that half of these deaths are due to 10 leading causes of death related to healthcare (viz., Ischemic heart disease, Covid-19, Stroke, Chronic obstructive pulmonary disease, lower respiratory infections, Trachea bronchus lung cancers, Alzheimer's disease and other dementias, Diabetes mellitus, Kidney disease and Tuberculosis). The pharmaceutical industry proves to be a precarious field playing a vital role in saving lives. It operates on continuous innovation and the adoption of new technologies to address global healthcare challenges and respond to medical emergencies. In the pharmaceutical industry, innovation is typically based on extensive research and development through various areas like manufacturing technology, packaging considerations, and customer-oriented marketing strategies.

The health and biotech sector is becoming progressively rich in data, which requires advanced analytical methods that can help understand the relationships within the data. However, the dearth of advanced technologies limits the drug discovery process, making it a time-consuming and expensive task. Artificial intelligence and machine learning can assist in overcoming these limitations by analysing biomedical data to find trends in biochemical features, discover new interactions between various chemicals, and generate predictions.

Artificial Intelligence is the most prominent and significant tool in the recent times. Artificial Intelligence has the potential to transform the drug discovery process. Discovering a new drug takes years and costs billions of dollars. AI can help streamline this process by analysing vast amounts of data and predicting which compounds will likely be effective. It can make drug discovery more efficient and more effective and benefit all parties involved ranging from companies developing new drugs to patients in desperate need of viable treatments.

AI has revolutionized numerous industries, and drug discovery is one among them. Recently it has emerged as a powerful tool in the search for new drugs. AI can speed up the drug discovery process, save expenses, and increase the success rate of new medication development.

THE ROLE OF AI IN ACCELERATING MEDICAL BREAKTHROUGHS

Artificial Intelligence (AI) also known as Deep Learning (DL), Machine Learning (ML), or Artificial Neural Networks (ANNs), has caught the attention and interest of people who work in medical technology. This is because a number of companies and big research labs have been working to make AI technologies ready for clinical use. These tools have the potential to improve care and patient turnover while also altering and enhancing the utility of practitioners.

PATIENT RECRUITMENT

Patient recruiting is one of the biggest obstacles in clinical studies. It can be challenging to find appropriate patients who fit certain requirements for a condition. Through the analysis of social media, electronic health records, and other data sources, AI-powered technologies can assist in identifying new patients and significantly reduce time and expense associated with patient recruiting.

PREDICTIVE ANALYTICS

Clinical trial data can be analyzed by AI systems to find patterns and forecast results. Researchers can use this to determine which therapies to continue and which to stop. Predictive analytics can also assist in spotting any safety concerns before they become serious ones.

DRUG DEVELOPMENT

AI can play a significant role in drug development. By analyzing large amounts of data it can identify potential drug targets and predict their efficacy. This can help researchers develop new drugs faster and more efficiently

REAL-TIME MONITORING

Real-time monitoring during clinical trials using AI-powered tools can help researchers identify potential safety issues early on and take appropriate action. As per USFDA (United States food and drug administration) using AI- tools can help researchers adjust treatment protocols based on patient responses (USFDA, 2018).

DATA ANALYSIS

Large amount of data from clinical trials can be analyzed by AI systems to find trends and patterns. As a result researchers may learn more about the causes of diseases and the effectiveness of treatments. Additionally, data analysis can be used to determine patient subgroups that would benefit more from particular treatments.

CONCLUSION

Due to the growing use of cutting-edge technology, advancements in clinical research, and the growing need for individualized care, the AI in healthcare market is expected to grow from USD 37.98 billion in 2025 to USD 674.19 billion by 2034, with a compound annual growth rate (CAGR) of 37.66% during the forecast period. Prominent pharmaceutical AI companies have dedicated time, funds, and resources to creating their custom AI solutions. Every solution is intended to upend the pharmaceutical sector on one hand while also resolving present issues simultaneously.

ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY SYSTEMS

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INTRODUCTION

Pharmaceutical research traditionally involves time-consuming experiments, high cost, and a significant probability of failure during clinical testing. AI addresses these challenges by shifting the industry toward data-driven, predictive, and automated methodologies. Machine learning (ML) and deep learning (DL) algorithms can identify patterns in biological and chemical data that humans cannot easily detect. These insights enable faster hypothesis generation, fewer laboratory trials, and improved decision-making.

AI further integrates with big data, robotics, and bioinformatics to support personalized medicine—allowing treatments to be designed based on a patient's genetics, lifestyle, and disease profile. Thus, AI is not just a supportive tool but a central driver in modern pharmaceutical innovation.

AI IN DRUG DEVELOPMENT AND FORMULATION

Accelerating Drug Discovery

The drug discovery process can take over a decade, but AI drastically shortens this timeline.

1. **Virtual screening:** AI screens millions of molecules in hours, predicting which compounds will bind effectively to a target protein.
2. **Deep learning models:** They evaluate molecular structures, toxicity, therapeutic potential, and metabolic pathways with high accuracy.
3. **Target identification:** AI analyzes genomic and proteomic databases to identify new biological targets for drug intervention, making precision medicine more achievable.
4. **Enhancing Formulation Design:** Formulation scientists use AI to predict the behaviour of excipients and active ingredients before performing laboratory work.

AI MODELS HELP IN:

1. Selecting the best polymers for sustained-release tablets,
2. Predicting solubility enhancement strategies for poorly soluble drugs,
3. Modeling pH-dependent stability,
4. optimizing particle size and flow properties,
5. Reducing batch failures by forecasting stability outcomes.
6. Machine learning also strengthens Design of Experiments (DoE) by reducing the number of trials required to reach an optimized, stable formulation



AI IN ADVANCED DRUG DELIVERY SYSTEMS

AI contributes heavily to developing innovative and precise drug delivery platforms.

NANOPARTICLES AND LIPOSOMAL SYSTEMS

AI predicts critical parameters such as particle size, drug-loading efficiency, zeta potential, and release kinetics. This ensures controlled and targeted delivery, especially in cancer therapy, where site-specific drug release can reduce toxicity.

PERSONALIZED DRUG DELIVERY

AI uses patient-specific data—genomics, disease biomarkers, metabolic rates—to customize dosage and delivery frequency. Devices like AI-driven insulin pumps monitor glucose in real time and automatically adjust insulin release, reducing complications.

MICRONEEDLES AND TRANSDERMAL SYSTEMS

AI MODELS PREDICT:

1. Penetration depth of microneedles,
2. Optimal geometry for painless drug delivery,
3. Skin permeability and biodistribution patterns.
4. This leads to more efficient non-invasive therapeutic systems.
5. Smart Implants and Wearables
6. AI-enabled implants and wearable technologies continuously monitor physiological signals such as temperature, enzyme levels, or heart rate. Based on these inputs, they release the drug in precise amounts, ensuring maximum therapeutic benefit with minimal side effects.
7. AI in Manufacturing and Quality Control
8. AI revolutionizes pharmaceutical manufacturing by making it safer, faster, and more efficient.
9. Automation & Real-Time Monitoring
10. AI-powered robots handle high-risk and repetitive tasks, ensuring sterility and precision.
11. Process Analytical Technology (PAT) supported by AI constantly monitors critical parameters during production—such as viscosity, particle size, and pressure—to maintain consistency.

PREDICTIVE QUALITY CONTROL

Computer vision systems detect defects such as tablet cracks, coating irregularities, or mislabelled packaging more accurately than human inspectors. Predictive maintenance algorithms also anticipate equipment failures, preventing downtime and reducing production cost.

CONCLUSION

AI is reshaping the pharmaceutical landscape through its powerful ability to analyze, predict, and optimize every stage of the drug lifecycle. From accelerating drug discovery to enabling smart drug delivery platforms and maintaining manufacturing quality, AI drives the development of safer, more effective, and personalized therapies. As AI continues to evolve and integrate with biotechnology, robotics, and biomedical engineering, it will lead the next era of pharmaceutical innovation—where treatments become smarter, faster, and truly patient-centered.

ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY SYSTEMS

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INTRODUCTION

Pharmaceutical technology has typically relied on experimental and iterative methods to develop or personalized treatment, and rising research costs have hastened the application of AI. AI algorithms excel at identifying patterns in enormous datasets, predicting outcomes, and automating labor-intensive activities, making them important across drug research and formulation science. Their application is quickly expanding—from early-stage molecular screening to advanced delivery platforms such as nano-formulations, smart implants, and controlled-release devices.

AI IN DRUG DISCOVERY AND PRE-FORMULATION STUDIES

Molecular Design and Target Identification Machine learning systems can screen millions of molecules in-silico, predicting biological activity, toxicity, and physicochemical behaviour with high accuracy. Deep generative models further assist in developing novel chemical structures optimised for drug-likeness, solubility, or target affinity.

Physicochemical and Pharmacokinetic Predictions AI models imitate solubility, permeability, stability, and metabolic pathways. Predictive techniques enable formulators to anticipate bad biopharmaceutical qualities early and adjust molecular architectures or delivery strategies accordingly. This minimizes experimental workload and shortens development timescales.

Automated Laboratory Tools Robotic systems led by AI optimize crystallization, salt selection, and compatibility screening. Closed-loop AI-robot platforms speed preformulation investigations and facilitate high-throughput experimentation.

AI IN PHARMACEUTICAL FORMULATION DEVELOPMENT

Predictive Modelling of Formulations ML methods such as random forests, support vector machines, and artificial neural networks predict formulation performance (e.g., dissolving rate, particle size, stability). These models integrate varied variables, from excipients characteristics to production parameters.

Optimization of Dosage Forms AI-driven design of experiments (AI-DOE) decreases the number of trials required to obtain optimal tablet hardness, disintegration, encapsulation efficiency, or controlled-release profiles. Formulations of tablets, injectables, liposomes, and polymeric systems benefit from computational optimization.

Quality-by-Design (QbD) Support AI enriches QbD frameworks by detecting critical material attributes (CMAs) and critical process parameters (CPPs), enabling real-time monitoring and predictive control. This enhances product uniformity and compliance with regulatory expectations.

AI IN ADVANCED DRUG DELIVERY SYSTEMS

Nanotechnology and Targeted Delivery AI assists in developing nanoparticles, micelles, dendrimers, and lipid systems with specified size, charge, and targeting ligands. Algorithms anticipate interactions with biological membranes, opsonisation rates, and circulatory behaviour.

Smart and Responsive Delivery Platforms AI enables creation of systems that respond to physiological stimuli (e.g., pH, glucose levels). Machine learning boosts sensor accuracy in implanted pumps or closed-loop insulin delivery, increasing patient outcomes.

Personalized Drug Delivery Patient-specific data—from genomics to wearable devices—feed AI systems that modify dosage, timing, and delivery route. Personalized inhalers, transdermal devices, and infusion pumps alter therapy dynamically depending on real-time feedback.

MANUFACTURING, QUALITY CONTROL, AND SUPPLY CHAIN APPLICATIONS

Automation and Process Control AI-enabled production lines use predictive maintenance, anomaly detection, and in-process monitoring to ensure product quality. AI facilitates continuous production, a developing trend in the pharmaceutical sector. Digital twins Digital twin technology mimics industrial processes virtually, allowing simulation of modifications without affecting output. AI models forecast deviations and determine ideal circumstances. Optimization of the supply chain AI increases logistics by anticipating demand, minimizing drug shortages, mitigating counterfeit concerns, and improving cold-chain management for vaccines and biologics.

CHALLENGES AND LIMITATIONS

- 1. Data Quality and Standardization** - AI models depend on large, clean, and interoperable datasets. Issues such as fragmentation, bias, and confidentiality can limit performance.
- 2. Regulatory and Ethical Considerations** - Regulatory agencies are developing guidelines for evaluating AI-based tools, but challenges persist in validation, algorithm transparency, and post-marketing surveillance.
- 3. Integration with Existing Systems** - Adoption requires training personnel and upgrading infrastructure. Smaller organisations may face cost and technical barriers.

FUTURE PERSPECTIVES

Deeper integration with multi-omics data, independent labs, and real-time clinical monitoring are key components of AI's future in pharmaceutical technology. Building trust and gaining regulatory approval will require Explainable AI (XAI). AI will enable more effective development pipelines, adaptive therapies, and ultra-personalized delivery systems when combined with developments in biology and materials science.

CONCLUSION

Artificial intelligence is transforming drug delivery and pharmaceutical technology by speeding up discovery, improving formulations, and facilitating individualized treatment plans. Despite ongoing difficulties, it has enormous promise to enhance productivity, accuracy, and patient outcomes. AI-driven advancements will be successfully translated into clinical and commercial applications if scientists, technologists, and regulators continue to collaborate.

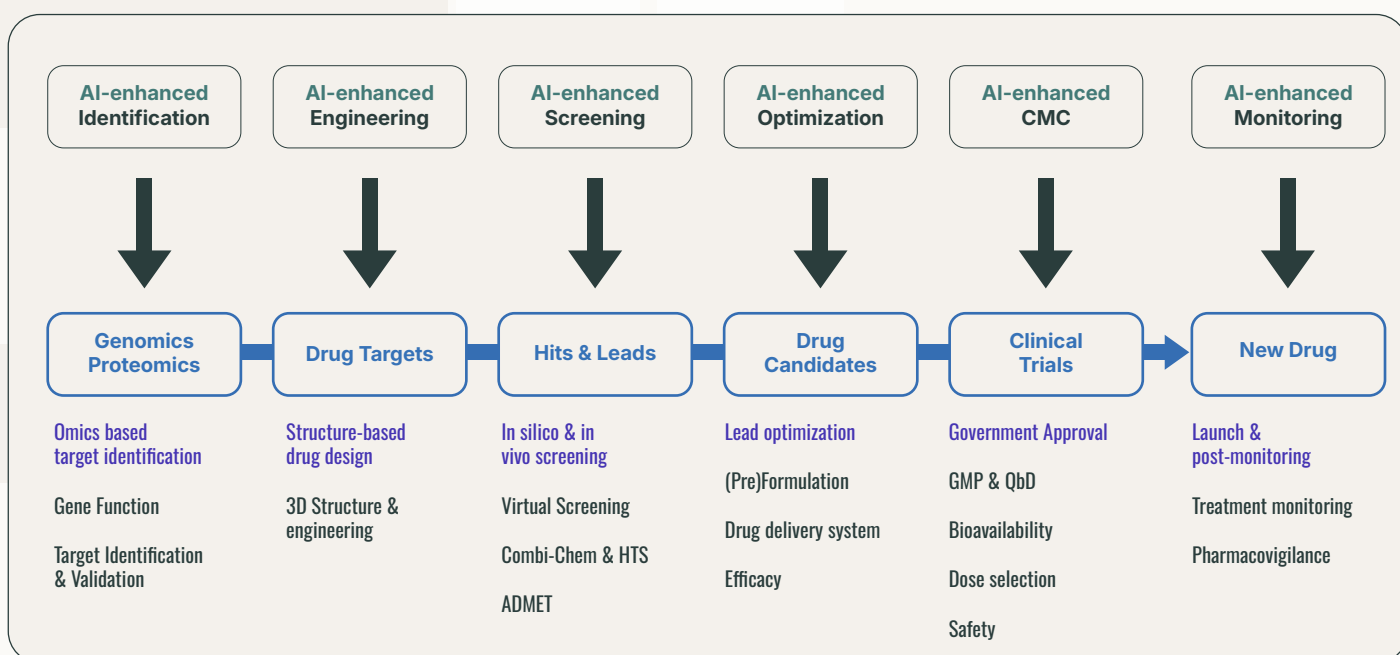
ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY DESIGN

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INTRODUCTION

The pharmaceutical industry is essential for addressing global healthcare challenges, including responding to emergencies such as the recent pandemic. The industry aims to develop new pharmaceutical innovations, from small drug molecules to biologics, with better stability and high potency to meet unmet disease treatment needs. However, addressing the significant levels of toxicity associated with new drugs remains a primary concern, requiring extensive research in the future. Despite advancements, the industry faces challenges and requires further technological developments to meet global medical and healthcare demands. Drug delivery technology has evolved remarkably, driven by the need to address ever-increasing challenges. AI imitates human behaviour in terms of the thought processes involved in problem-solving. The pharmaceutical business has a genuine opportunity to change how it does research and development (R&D), making it more effective and dramatically raising the success of early drug development with the use of artificial intelligence (AI) and machine learning. Artificial intelligence achieves this by employing Natural Language Processing to convert spoken language from humans into a language that computers can comprehend. Deep learning is also a requirement for AI to finish this assignment. By analysing huge quantities of data and identifying new or recurring patterns in the data, AI trains computers to carry out certain tasks with the least amount of human participation. AI play a very crucial role in drug process and formulation of new drug delivery as show in following image, as following,



THE NEED OF ASSISTIVE GENERATIVE AI IN SEMICONDUCTOR DESIGN AND MANUFACTURING

DESIGN

Innovative EDA Tool Can Speed Up The Process of Design Development. It Can Be Done By GenAI Taking Over The Repetitive Tasks.

MANUFACTURING

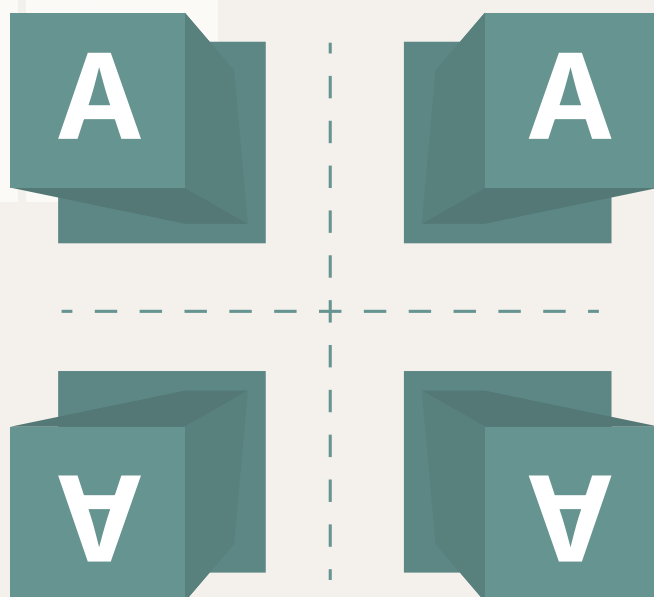
GenAI Can Help Generate Defects That Can Occur With Ultra-Advanced Semiconductor Nodes. Enabling Better Process Control And Yield Management.

TIME

Based On Historical Data, GenAI Can Improve The Design And Manufacturing Process And Help Semiconductor Engineers Iterate Faster Than Ever.

COST

GenAI Can Reduce The Design And Manufacturing Time, Which Can Potentially Open Avenues To Bring Cost Benefits.



AI TOOLS USED IN PHARMA

A growing number of specialized AI tools and platforms are being utilized by pharmaceutical companies to address specific needs in drug discovery and portfolio management. Insilco Medicine offers its Pharma.AI Suite, which includes tools like Panda Omics for target discovery and Chemistry42 for molecule generation, demonstrating significant strides in accelerating drug discovery.

S. No.	AI/ML models	Description/Usage
1	Generative Adversarial Networks (GANs)	GANs are widely used in drug product development to generate novel chemical structures and optimize their properties. GANs consist of a generator network that creates new molecules and a discriminator network that evaluates their quality, leading to the generation of structurally diverse and functionally optimized drug candidates
2	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. They capture sequential dependencies and can generate new sequences based on learned patterns.
3	Convolutional Neural Networks (CNNs)	CNNs are effective in image-based tasks, including analyzing molecular structures and identifying potential drug targets. They can extract relevant features from molecular images and aid in drug design and target identification

S. No.	AI/ML models	Description/Usage
4	Long Short-Term Memory Networks	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.
5	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. They can extract useful information from scientific literature, patent databases, and clinical trial data, enabling researchers to make informed decisions in drug development.
6	Reinforcement Learning (RL)	RL techniques have been applied to optimize drug dosing strategies and develop personalized treatment plans. RL algorithms learn from interactions with the environment to make sequential decisions, aiding in dose optimization, and improving patient outcomes.
7	Bayesian Models	Bayesian models, such as Bayesian networks and Gaussian processes, are employed for uncertainty quantification and decision-making in drug development. They enable researchers to make probabilistic predictions, assess risks, and optimize experimental designs
8	Deep Q-Networks (DQNs)	DQNs, a combination of deep learning and reinforcement learning, have been used to optimize drug discovery processes by predicting the activity of compounds and suggesting high-potential candidates for further experimentation.
9	Autoencoders	Autoencoders are unsupervised learning models used for dimensionality reduction and feature extraction in drug development. They can capture essential characteristics of molecules and assist in compound screening and virtual screening.
10	Graph Neural Networks (GNNs)	GNNs are designed to process graph-structured data, making them suitable for drug discovery tasks that involve molecular structures. They can model molecular graphs, predict properties, and aid in virtual screening and de novo drug design.
11	Panda Omics	target discovery
12	Atom wise	Uses convolutional neural networks (CNNs) to identify potential drug candidates by analysing molecular interactions.
13	Chemistry42	for molecule generation.
14	Ex Scientia	Developed an AI-led drug design platform that has been used in collaborations with major pharmaceutical companies.
15	DeepMind's AlphaFold	Predicts protein structures, crucial for understanding biological processes and identifying drug targets.
16	Cure Metrix stands	Stands at the forefront, employing AI to predict adverse drug events with remarkable accuracy and foresight.

S. No.	AI/ML models	Description/Usage
17	Janssen's Trials360.ai	Optimizes clinical trial design and improves patient care.
18	Averroes.ai	Provides real-time anomaly detection in manufacturing processes for quality control.
19	Iktos	Offers Makya for de novo drug design and Spaya for synthesis planning.
20	Cline Rion	Uses AI to improve patient recruitment by analysing real-time hospital data.

APPLICATION OF ARTIFICIAL INTELLIGENCE:

Artificial Intelligence in the Pharmaceutical Industry is revolutionizing every aspect of the sector, from drug discovery and development to manufacturing and marketing. Artificial intelligence (AI) is transforming pharmaceutical technology and drug delivery design by enhancing efficiency, accelerating processes, and enabling the creation of more effective and personalized treatments.

1. DRUG DISCOVERY AND DEVELOPMENT:

Target Identification: AI algorithms analyse vast biological datasets to pinpoint potential drug targets associated with diseases.

Virtual Screening: AI efficiently screens large chemical libraries, predicting which compounds are likely to bind to specific targets and prioritizing promising drug candidates.

De Novo Drug Design: Generative AI models design entirely new drug-like molecules with desired properties, expanding the chemical space for exploration.

Preclinical Testing: AI can help predict drug behaviour in preclinical models, reducing the need for extensive animal testing.

Clinical Trial Optimization: AI can improve clinical trial design, patient selection, and data analysis, leading to faster and more efficient trials.

2. DRUG FORMULATION AND DELIVERY

Predictive Modelling: AI can predict the optimal composition of drug delivery systems by analysing data on excipients, active pharmaceutical ingredients, and their interactions.

Excipients Selection: AI can help identify the most suitable excipients to enhance drug stability, bioavailability, and patient compliance.

Dosage Form Optimization: AI algorithms can optimize tablet and capsule formulations, considering factors like drug release, disintegration, and dissolution.

Nanoparticles-based Delivery: AI can assist in designing and optimizing nanoparticles-mediated drug delivery systems, including targeted drug delivery and biomarker sensing.

3. PERSONALIZED MEDICINE AND TARGETED DELIVERY

Individualized Treatment Plans: AI can analyse patient data (genetics, medical history, etc) to recommend personalized drug combinations and dosages.

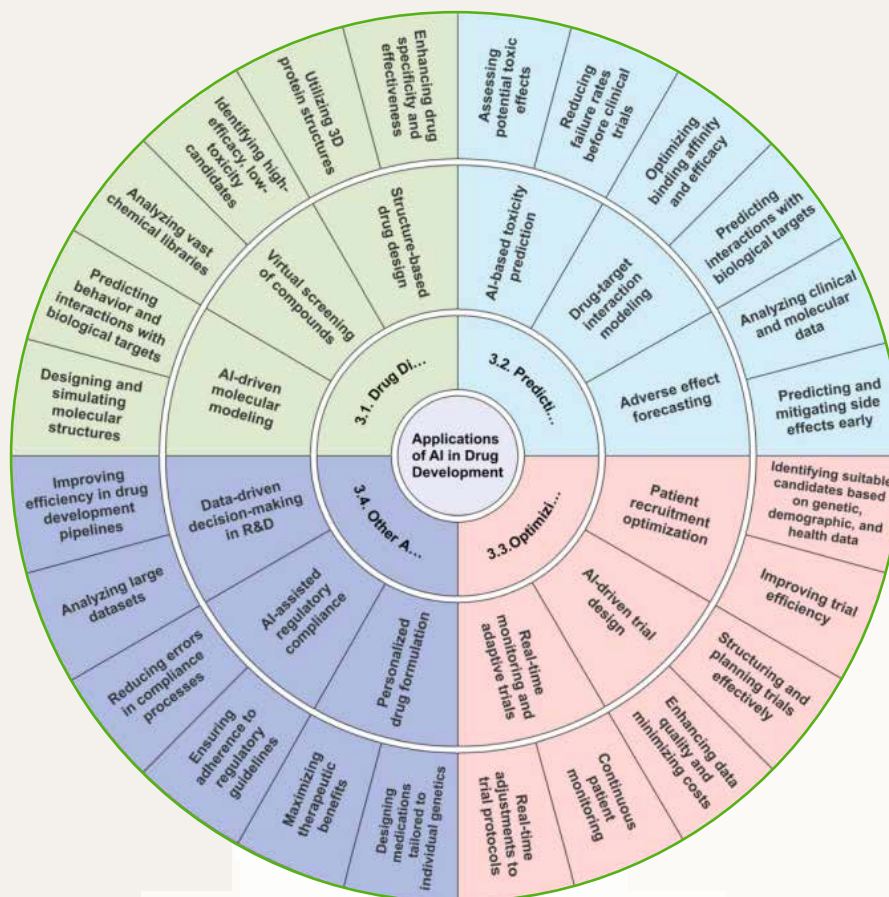
Targeted Drug Delivery: AI can help design drug delivery systems that target specific tissues or cells, minimizing side effects and maximizing therapeutic effect.

Biomarker Detection: AI can be integrated with nanoparticles to detect biomarkers and ensure accurate drug delivery to the affected area.

4. MANUFACTURING AND SUPPLY CHAIN:

Pharmacovigilance: AI can analyse adverse event data and identify potential drug safety signals.

Regulatory Submissions: AI can automate the creation of regulatory documents, speeding up the approval process.



CONCLUSION

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. Overall, the integration of AI technologies holds great promise for accelerating drug development, technology and revolutionizing the pharmaceutical industry, promoting its evolution from era 4.0 to era 5.0. Although AI had some challenges, including data privacy concerns, the need for high-quality datasets, and the requirement for interdisciplinary expertise, which needs more focus in future.

ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY SYSTEM

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INTRODUCTION

The pharmaceutical industry is undergoing a major digital revolution. Traditional drug development is expensive, time-consuming and often inefficient, with high failure rates. Artificial intelligence provides an opportunity to accelerate decision-making, reduce trial-and-error experimentation and enhance precision. The integration of machine learning (ML), deep learning (DL), neural networks and predictive analytics supports innovation across pharmaceutical technology and advanced drug delivery systems.

1. ROLE OF AI IN DRUG DISCOVERY AND PREFORMULATION

One of the most established applications of AI is in the pre-formulation and formulation stages.

Prediction of Physicochemical Properties: AI models (e.g., QSAR - Quantitative Structure-Activity Relationship) predict solubility, permeability, and stability of drug candidates, reducing the need for extensive physical testing.

Excipients Selection: Algorithms analyze historical data to recommend the optimal combination of excipients (binders, disintegrates) that ensure drug stability and bioavailability.

Design of Experiments (DoE): AI automates the DoE process, simultaneously varying multiple parameters (e.g., temperature, mixing speed) to find the "sweet spot" for formulation stability much faster than traditional. AI in statistical methods.

1. ROLE OF AI IN DRUG DISCOVERY AND PREFORMULATION

The precision of AI is particularly valuable in designing complex delivery systems where slight variations can drastically alter efficacy.

1- Nanomedicine and Nanoparticles: Developing Nanoparticles (liposomes, polymeric Nanoparticles) involves tuning size, surface charge (zeta potential), and drug entrapment efficiency.

Optimization: Artificial Neural Networks (ANNs) are widely used to predict the particle size and release kinetics of Nanoparticles based on input variables like polymer concentration and stirring speed.

Targeting: AI helps design surface modifications (e.g., attaching ligands) that allow Nanoparticles to specifically target cancer cells while sparing healthy tissue, minimizing side effects.

2- Personalized Medicine (3D Printing) AI is the backbone of personalized drug delivery, particularly in 3D printed pharmaceuticals.

Dosage Customization: ML algorithms analyze patient-specific data (genetics, age, weight) to calculate the precise dosage required. **Printability Prediction:** AI predicts the "printability" of drug-ink formulations, ensuring that the 3D printer creates a tablet with the correct structural integrity and dissolution profile. speed.

3. Smart Manufacturing and Quality Control: Beyond the lab, AI is revolutionizing the factory floor through Process Analytical Technology (PAT).

Real-time Monitoring: Computer vision and sensors monitor the manufacturing line in real-time. If a batch of tablets shows a deviation (e.g., unexpected colour change or crumbling), AI systems can instantly adjust process parameters to correct it, reducing waste.

Predictive Maintenance: AI predicts when critical machinery (e.g., tablet presses, lyophilizers) will fail, preventing costly production downtime.

4. Challenges and Future Perspectives: Despite the progress, significant hurdles remain

Data Quality (The "Black Box" Problem): AI models are only as good as the data they are fed ("Garbage In, Garbage Out"). Historical pharmaceutical data is often siloed, unstructured, or proprietary.

Regulatory Hurdles: Regulatory bodies like the FDA and EMA are still developing frameworks for "AI as a Medical Device" (SaMD). Approving a drug developed by a "black box" algorithm where the decision-making process isn't fully transparent remains a challenge.

Skill Gap: There is a critical need for workforce development. The industry requires professionals who are hybrid experts in both pharmaceutical sciences and data science.

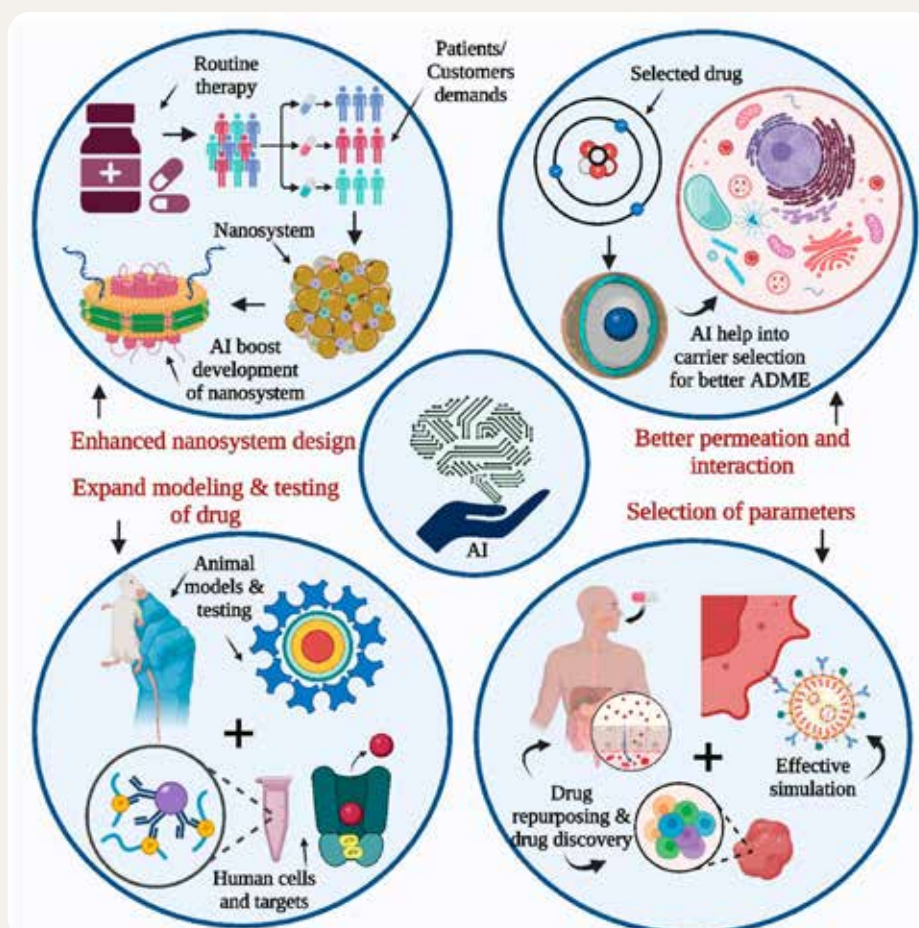


Fig:1 various phases of New drug development

CONCLUSION

AI is not merely a tool but a fundamental paradigm shift in pharmaceutical technology. By enabling the design of "smart" drug delivery systems—from self-regulating insulin pumps to tumour-seeking Nanoparticles—AI is moving the field toward an era of hyper-personalized, efficient, and safer medicine. Future success depends on interdisciplinary collaboration and the establishment of robust regulatory standards for AI-generated health solutions.

COMPARISON OF TRADITIONAL AND AI-ASSISTED APPROACHES IN PHARMA

AI-assisted Pharma drastically speeds up and cuts costs in drug discovery, clinical trials, and manufacturing (years to months, huge savings) by using predictive models for molecules, patient selection, and quality control, while traditional methods rely on slow, expensive, often subjective trial-and-error, but AI introduces challenges like data bias and ethics, requiring careful validation.

HERE'S A DETAILED COMPARISON:

Traditional Approaches

- **Methodology:** Relies on manual lab work, human expertise, periodic monitoring, and known statistical models (like FMEA, HACCP).
- **Speed:** Very slow; drug development takes 10-15 years.
- **Cost:** Extremely high (billions per drug); early design costs are significant.
- **Data Analysis:** Limited by human capacity; periodic, often subjective data collection.
- **Risk Management:** Reactive, often subjective, and less scalable.
- **Success Rate:** Lower; traditional methods yield lower success rates in identifying viable drug candidates.

AI-Assisted Approaches

- **Methodology:** Uses machine learning (ML) for predictive modelling, automation, and pattern recognition (e.g., Deep Learning for protein structures, digital biomarkers).
- **Speed:** Significantly faster; can reduce timelines by 50-80% in R&D, clinical trials, and production.
- **Cost:** Lower; can cut R&D and clinical trial costs by 40-70%.
- **Data Analysis:** Real-time, automated, advanced analysis of complex, high-dimensional data.
- **Risk Management:** Proactive, predictive, real-time, and more accurate.
- **Success Rate:** Higher; AI models predict toxicity and efficacy better, increasing success rates for clinical candidates.

Key Areas of Transformation

- **Drug Discovery:** AI identifies promising compounds and predicts properties (ADMET) faster and more accurately, reducing failed candidates.
- **Clinical Trials:** AI optimizes patient recruitment, monitors outcomes continuously (digital biomarkers), and predicts adverse events, shortening trials.
- **Formulation:** AI predicts optimal excipients and release rates, streamlining formulation development.
- **Quality Control (QC):** AI-driven models predict deviations, boost productivity, and reduce lab lead times in manufacturing.

Challenges with AI

Requires massive, high-quality data sets, faces data integration hurdles, and raises privacy/ethical concerns.

Risk of bias from under represented data and the need for careful validation of AI predictions.

In essence, AI shifts Pharma from slow, manual, and reactive processes to rapid, data-driven, and predictive models, fundamentally changing timelines, costs, and success potential.

ARTIFICIAL INTELLIGENCE IN PHARMACEUTICAL TECHNOLOGY AND DRUG DELIVERY DESIGN

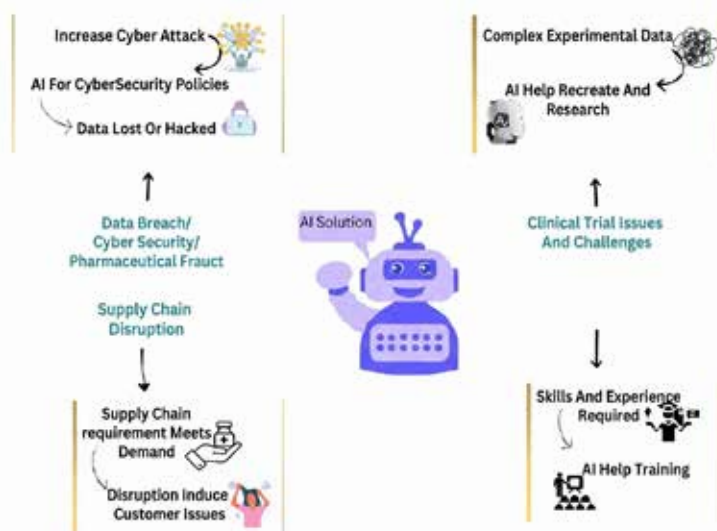
DR. RAKESH JATAV, MS. ANUBHA JAIN

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INTRODUCTION

Numerous industries are striving to enhance their progress to meet the demands and expectations of their customers, utilizing various methodologies. The pharmaceutical industry is a critical field that plays a vital role in saving lives. It operates based on continuous innovation and the adoption of new technologies to address global healthcare challenges and respond to medical emergencies, such as the recent pandemic. In the pharmaceutical industry, innovation is typically predicated on extensive research and development across various domains, including but not limited to manufacturing technology, packaging considerations, and customer-oriented marketing strategies. The industry aims to develop new pharmaceutical innovations, from small drug molecules to biologics, with better stability and high potency to meet unmet disease treatment needs. However, addressing the significant levels of toxicity associated with new drugs remains a primary concern, requiring extensive research in the future.

The industry aims to develop new pharmaceutical innovations, from small drug molecules to biologics, with better stability and high potency to meet unmet disease treatment needs. However, addressing the significant levels of toxicity associated with new drugs remains a primary concern, requiring extensive research in the future. Due to supply chain disruptions, the pharmaceutical industry has significantly impacted customer satisfaction, corporate reputation, and potential profits. The healthcare sector has a continuing need for skilled workers, which makes it necessary to provide healthcare staff with ongoing training to increase their participation in normal tasks. Within the pharmaceutical sector, determining skill shortages in the workplace is an essential task. The implementation of AI is poised to bring about a significant transformation in the way the pharmaceutical industry handles supply chain operations. It also consolidates numerous AI research endeavors from recent decades to create effective solutions for diverse supply chain issues. Additionally, the study suggests potential research areas that could enhance decision-making tools for supply chain management in the future.



CURRENT PHARMACEUTICAL SITUATION AND THE ROLE OF AI

Because of its many benefits, continuous research on small molecules in the pharmaceutical sector improves goods and raises customer satisfaction. The creation of synthetic derivatives is economical, and the chemical synthesis procedure is straightforward. As a result, the pharmacy industry offers a wide variety of stable and effective small-molecule-loaded formulations. However, generic molecules compete with numerous novel small compounds, and their introduction necessitates intricate data and clinical trials, especially when treating rare disorders. These procedures put financial pressure on businesses to prioritize innovation. However, in order to counteract the crises brought on by the small size of molecules and the restricted distribution of research and discoveries, the biomolecular medication industry is growing. The shape and reactivity of small molecules dictate their functions. Biomolecules, on the other hand, are bigger units that are primarily composed of nucleotides or ribonucleotides for nucleic acids and amino acids from the protein source. The supramolecular sequence and spatial conformation also affect their stability and function. Successful biomolecule-based products include adalimumab and insulin. These compounds have complicated pharmacokinetic properties, and the most popular and preferred method of delivery is infusion. Molecular stabilization and pharmacokinetic modulation are crucial components of nucleic acid-based research. New technical developments may help with these difficulties and associated problems. Achieving pharmacokinetic exposure and improving these molecular forms are important objectives. AI still has substantial limitations that necessitate human interaction to interpret complex data, despite its great potential in drug delivery innovation and drug discovery. Datasets play a major role in AI predictions, but human interaction is necessary for result interpretation, especially in cases that are unclear, in order to arrive at the right conclusions. AI faces difficulties in processing data for predictions due to algorithmic bias and the evaluation of hypotheses. Furthermore, inactive molecules might be found by docking simulations. Therefore, in order to remove system bias concerns, human engagement is necessary for successful decision-making and cross-verifications. However, AI has the potential to be used, and more research could lessen its drawbacks and improve its efficiency and dependability.

OVERVIEW OF ARTIFICIAL INTELLIGENCE MODELS UTILIZED IN PHARMACEUTICAL SCIENCES

Different AI models, each with unique capabilities and applications, are used in pharmaceutical sciences for a variety of reasons. In this discipline, machine learning models—like supervised learning—are essential. In supervised learning, models are trained on labeled datasets to provide predictions or judgments. Commonly employed methods include decision trees, support vector machines (SVM), and regression models. Different AI models, each with unique capabilities and applications, are used in pharmaceutical sciences for a variety of reasons. In this discipline, machine learning models—like supervised learning—are essential. In supervised learning, models are trained on labeled datasets to provide predictions or judgments. Commonly employed methods include decision trees, support vector machines (SVM), and regression models.

ARTIFICIAL INTELLIGENCE IN MEDICINAL CHEMISTRY

1. By providing new opportunities

for drug design, synthesis, and optimization, artificial intelligence's incorporation into medicinal chemistry represents a substantial advancement over conventional pharmaceutical discovery techniques. These are made possible by artificial intelligence, which processes enormous volumes of data, forecasts molecular behaviors, and more accurately and quickly simulates drug interactions. In-depth discussion of AI's function in medicinal chemistry and its effects on the discipline will be covered in this section. These are made possible by artificial intelligence, which processes enormous volumes of data, forecasts molecular behaviors, and more accurately and quickly simulates drug interactions. This section will examine AI's function in medicinal chemistry in greater detail as well as its effects on the area. These are made possible by artificial intelligence, which processes enormous volumes of data, forecasts molecular behaviors, and more accurately and quickly simulates drug interactions. In-depth discussion of AI's function in medicinal chemistry and its effects on the discipline will be covered in this section.

2. Structure-Activity Relationships

Designing compounds with targeted therapeutic effects and few adverse effects is made easier by artificial intelligence models that forecast the relationship between chemical structures and biological activity. By identifying important structural characteristics that affect biological activity, these models aid in the improvement of lead compounds.

3. Synthesis Prediction and Optimization

By predicting effective synthetic pathways, artificial intelligence lowers the resources needed for drug manufacture. It streamlines the entire drug development process by predicting reaction outcomes and identifying new synthesis routes.

4. Molecular Docking and Pharmacophores

Artificial intelligence facilitates Pharmacophores discovery and molecular docking by simulating interactions between pharmaceuticals and biological targets. This aids in the identification of novel compounds with desired biological properties.

5. Predictive Absorption, Distribution, Metabolism, Excretion, and Toxicity Modeling

Drug discovery relies heavily on the ability to predict ADMET (absorption, distribution, metabolism, excretion, and toxicity) features. By offering precise forecasts, which are crucial for determining the drug-likeness and prospective success of novel compounds, artificial intelligence greatly helps in this field. Predictive ADMET modeling is covered in full in the "Predictive ADMET and PK/PD Modeling" subsection under "AI in Pharmacology and Toxicology."

6. Quantitative Structure-Activity Relationship Models

Quantitative structure-activity relationship (QSAR) models powered by artificial intelligence forecast a compound's activity based on its chemical structure, which is essential for selecting compounds that show promise for more research.

ARTIFICIAL INTELLIGENCE IN MEDICINAL CHEMISTRY

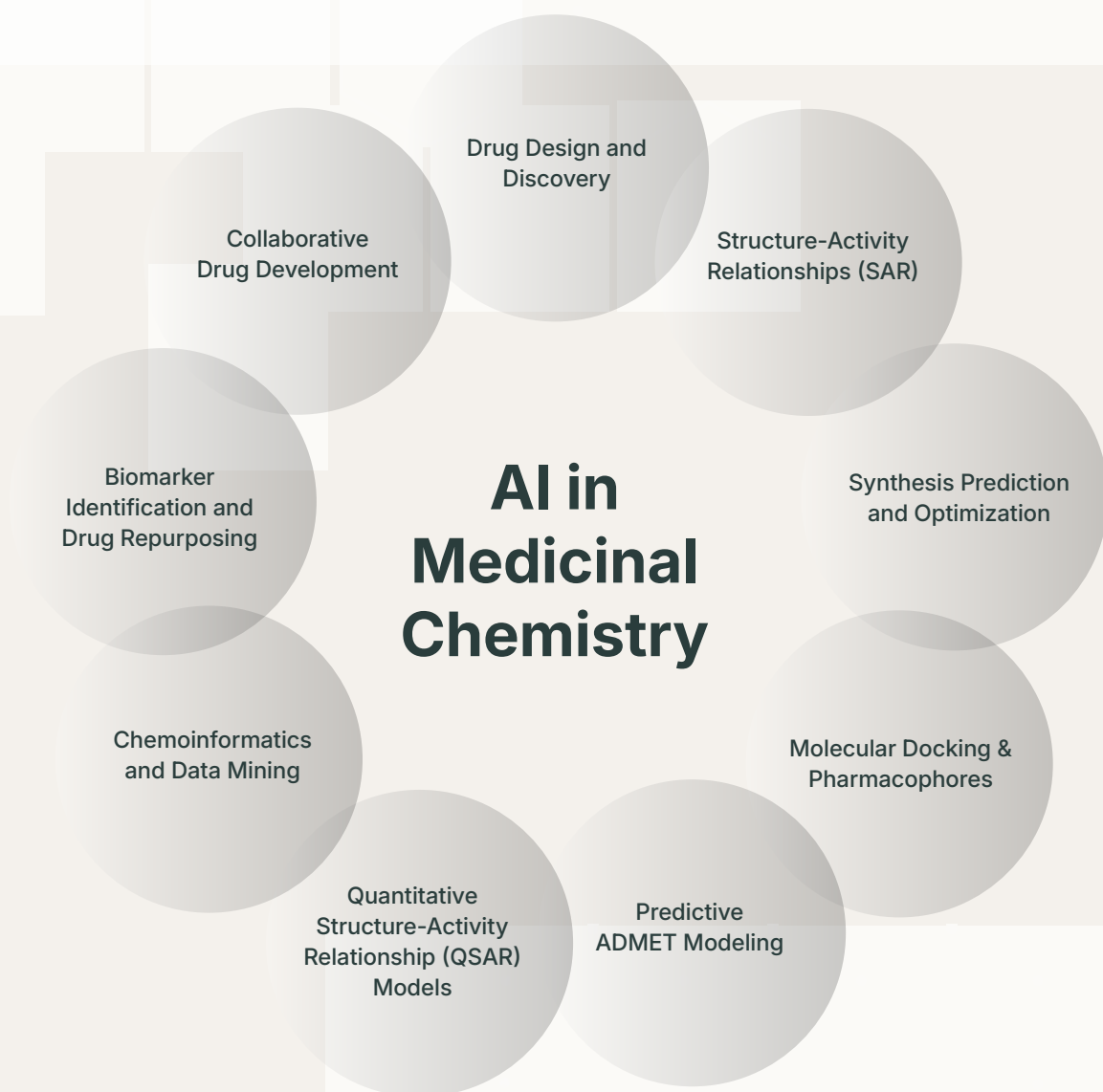


Fig.2 Role of artificial intelligence (AI) in medicinal chemistry

AI MODELS USED IN PHARMACEUTICAL INDUSTRIES

AI/Machine Learning Models	Description/Usage
GenerativeAdversarial Networks (GANs)	In order to create new chemical structures and enhance their characteristics, GANs are frequently utilized in the production of pharmaceutical products. GANs produce structurally varied and functionally optimized drug candidates by combining a discriminator network to assess the quality of the novel molecules produced by the generator network.
Recurrent Neural Networks (RNNs)	RNNs are frequently used in drug development for sequence-based tasks such peptide sequence design, genetic data analysis, and protein structure prediction. They record sequential relationships and have the ability to create new sequences using patterns it has learnt.

AI/Machine Learning Models	Description/Usage
Convolutional Neural Networks (CNNs)	CNNs work well for image-based applications like finding possible drug targets and analyzing chemical structures. They can help with target discovery and drug design by extracting pertinent information from molecular pictures.
Long Short-Term Memory Networks (LSTMs)	One kind of RNN that is particularly good at modeling and forecasting temporal relationships is called an LSTM. They have been employed to forecast drug concentration-time profiles and assess drug efficacy in pharmacokinetics and pharmacodynamics investigations.
Transformer Models	In the pharmaceutical industry, transformer models—like the well-known BERT (Bidirectional Encoder Representations from Transformers) model—have been used for natural language processing tasks. They are able to extract valuable information from clinical trial data, patent databases, and
Reinforcement Learning (RL)	Personalized treatment regimens and drug dosage optimization have been achieved through the use of RL methods. In order to make sequential judgments that help with dose optimization and enhance patient outcomes, RL algorithms learn from interactions with the environment.
Bayesian Models	In drug development, Bayesian models—like Bayesian networks and Gaussian processes—are used to quantify uncertainty and make decisions. They help researchers evaluate risks, optimize experimental designs, and make probabilistic predictions.
Deep Q-Networks (DQNs)	By forecasting a compound's activity and recommending high-potential candidates for more research, DQNs—a hybrid of deep learning and reinforcement learning—have been utilized to improve drug discovery procedures.
Auto encoders	In drug development, auto encoders are unsupervised learning models that are utilized for feature extraction and dimensionality reduction. They can help with compound and virtual screening by capturing key properties of compounds.
Graph Neural Networks (GNNs)	Because GNNs are made to handle graph-structured data, they can be used for molecular structure-based drug discovery activities. They can help with virtual screening and de novo drug creation; anticipate characteristics, and model molecular graphs.

AI FOR DRUG DISCOVERY

In many respects, artificial intelligence has transformed drug development and discovery. The following are a few of AI's major contributions in this field:

1. Target Identification

AI algorithms are able to find possible therapeutic targets by analyzing a variety of data sources, including clinical, proteomic, and genomic data. AI aids in the development of drugs that can alter biological processes by identifying targets and molecular pathways linked to disease.

2. Virtual Screening:

AI makes it possible to efficiently screen enormous chemical libraries in order to find therapeutic candidates with a high probability of attaching to a particular target. AI assists researchers in prioritizing and choosing by modelling chemical interactions and forecasting binding affinities.

3. Structure-Activity Relationship (SAR) Modelling

Artificial intelligence models are able to connect a compound's chemical makeup to its biological action. Because of this, scientists can create compounds with desirable properties including high potency, selectivity, and favourable profiles of pharmacokinetics.

4. De Novo Drug Design

Artificial intelligence algorithms can suggest new chemical compounds that resemble drugs by using generative models and reinforcement learning. AI broadens the chemical space and facilitates the creation of novel drug candidates by learning from chemical libraries and experimental data.

5. Optimization of Drug Candidates

AI systems are able to evaluate and improve medication candidates by taking into account a number of variables, such as pharmacokinetics, safety, and efficacy. This aids scientists in optimizing therapeutic compounds to maximize efficacy and reduce adverse effects.

6. Drug Repurposing

Large-scale biomedical data can be analyzed using AI approaches to find current medications that may be useful in treating various illnesses. AI speeds up the drug discovery process and lowers costs by repurposing current medications for new applications.

7. Toxicity Prediction

By examining the chemical makeup and properties of molecules, artificial intelligence (AI) algorithms are able to forecast the toxicity of drugs. Toxicological databases can be used to train machine learning algorithms that can detect dangerous structural characteristics or predict negative effects. This aids researchers. Give priority to safer substances and reduce the possibility of negative clinical trial reactions.

CONCLUSION

Drug delivery systems are being revolutionized by AI, which makes tailored, adaptive, and targeted treatments possible. Pharma researchers and medical professionals can increase drug efficacy, reduce adverse effects, and improve patient outcomes by utilizing AI's strengths in data analysis, pattern identification, and optimization. Pharmacokinetics and pharmacodynamic have undergone a revolution thanks to AI-based techniques. Compared to conventional experimental techniques, they have a number of benefits. Predicting pharmacokinetic characteristics, simulating drug distribution and clearance in the body, and optimizing medication dosage and administration routes are all possible with AI-based models. AI-based computational techniques for PBPK models can streamline their creation and optimize their parameters, negating the necessity for clinical trials on humans and animals. Big data and artificial intelligence (AI) enable computational pharmaceuticals, which transforms the drug distribution process by offering a more effective, economical, and data-driven method. It makes it possible to optimize medication formulations, provide individualized treatments, comply with regulations, and lower risk, all of which eventually improve patient results and drug manufacturing procedures. As a whole, the incorporating AI technologies has enormous potential to transform the pharmaceutical sector, propel it from era 4.0 to era 5.0, speed up medication development, and enhance patient outcome²

ABOUT

SAGAR GROUP, SIPTec AND SIPTec-R

Sagar group came into existence in the year 1983 under the visionary leadership of Chairman Shri Sudhir Kumar Agrawal. Over the years, it has now transformed into one of the largest corporate house and business conglomerate of Central India. In its journey of over three decades, the group has successfully ventured in the field of education, real estate, production and manufacturing to employ 5000+ people and impact lives of more than two lakh people every day.

Sagar Group has been felicitated with IBC24 Excellence Award 2017 for its contribution to Madhya Pradesh's Industrial Development and Incredible Societal Development.

Agrawal Builders have established its presence as one of the leading *Real Estate giants with over 40 years of rich experience in building state-of-art residential projects.*

Sagar Manufacturers Pvt Ltd has pledged to use the best fibers to produce superior quality yarns with the world-class production technology. In a short span of time the company has achieved an installed *capacity of 2,00,000 spindles and exporting its products to over 20+ countries.*

Sagar Nutriments Pvt Ltd is Sagar Group's recent venture in food processing premium quality basmati rice.

Sagar Group has earned a lot of praise across the nation empowering youth of Madhya Pradesh with a bright career and life. The group provides world class school and technical education under **Sagar Group of Institutions** to 20000+ students with 2000+ dedicated faculties. The group imparts schooling through the chain of **Sagar Public Schools (SPS)** to nurture the young mind. Today, SPS is considered as the most preferred brand for holistic education and Indian Value System to its core featuring amongst the **Top 100 schools in India** with its campuses at Saket Nagar, Gandhi Nagar, Rohit Nagar, Ratibad, Katara Extension and Dwarka Dham. Sagar Institutes (SISTec) are engaged in providing the best technical education in the field of engineering, pharmacy, and management.

Sagar Institute of Pharmacy and Technology (SIPTec) is the premier institution known for its high standards in teaching and research in pharmaceutical sciences. SIPTec was established in 2008. The Institute is also registered under CCSEA. Today, within a short span of 15 years, the institute has gained a reputation of being one of the **top Pharmacy Colleges in MP** that provides total pharmaceutical education comprising B.Pharm and M.Pharm (Pharmaceutics & Pharmaceutical Chemistry).

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