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### Artificial Intelligence in Drug Discovery and Development: Current Status, Challenges and Future Prospects

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**Abstract:** The review article examines the transformative influence of Artificial Intelligence (AI) in redefining the paradigms of drug discovery and pharmaceutical development. It explores how progressive innovations in AI methodologies including Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP), Reinforcement Learning (RL), Graph Neural Networks (GNN), and Generative AI are being strategically harnessed to address critical bottlenecks in the drug development continuum. Key areas of focus include target identification, lead molecule exploration, rational drug design, optimization strategies, and clinical trial orchestration. The review highlights AI's potential to revolutionize the pharmaceutical landscape by expediting drug discovery trajectories and curtailing the costs associated with introducing novel therapeutic entities.

**Keywords:** Artificial intelligence, Preformulation, Drug discovery, Optimization, Drug development, Machine learning

#### 1. INTRODUCTION

Artificial Intelligence (AI) refers to the broad discipline that encompasses the minimal human involvement required for a computer system to emulate intelligent behaviors. It constitutes a specialized domain within computer science dedicated to developing programs that address complex problems (1). Every stage of the pharmaceutical product life cycle, including drug discovery, optimization, formulation development, characterization, quality testing, marketing and post marketing – surveillance, can integrate AI to improve its efficacy (2). The advent of Artificial Intelligence (AI) has emerged as a transformative catalyst within the biomedical and pharmaceutical landscape. AI driven methodologies are being strategically harnessed to mitigate critical bottlenecks in drug discovery and development optimize patient outcomes and reinforce the efficiency of health care delivery framework (3).

This review elucidates the transformative influence of Artificial Intelligence (AI) in redefining paradigms of drug discovery and pharmaceutical development. The investigation delineates the manner in which progressive innovations in AI methodologies encompassing Machine Learning (ML), Deep Learning (DL), Natural Language Processing (NLP), Reinforcement Learning (RL), Graph Neural Network (GNN) and Generative Artificial Intelligence (Gen- AI), are being strategically harnessed to confront critical bottlenecks within the drug development continuum. These include the domains of target identification,

lead molecule exploration rational drug design, optimization strategies and clinical trial orchestration. Furthermore, the review prognosticates the prospective potential of AI to revolutionize the pharmaceutical landscape by expediting the drug discovery trajectory, curtailing probability of successful market introduction of novel therapeutic entities (4).

## **1.AI in Preformulation Research**

Preformulation refers to the systematic characterization of a drug substance's physicochemical attributes to inform and optimize formulation design, representing a critical and foundational phase in pharmaceutical product development. During this stage, potential formulation-related challenges including inadequate aqueous solubility, chemical or physical instability and incompatibilities between the active pharmaceutical ingredient and excipients are proactively identified and addressed (5). Although conventional preformulation methodologies have demonstrated reliability, they are often associated with substantial financial costs, extended timelines and intensive labour requirements. The integration of artificial intelligence into Preformulation investigation offers a robust and innovative alternative, enabling enhanced predictive precision, efficient utilization of limited material resources, and significant acceleration of formulation development workflows (6).

### **1.1.Physicochemical property**

A key application of artificial intelligence in preformulation studies involves the use of quantitative structure-activity relationship (QSAR) models and machine learning algorithms to forecast the physicochemical characteristics of molecules. These models, which include techniques like Support Vector Machines (SVM), Random Forests (RF), and Artificial Neural Networks (ANNs), correlate molecular descriptors with a compound's behavior to predict attributes such as melting point, pKa, solubility, and logP (7). Notably, these computational methods have demonstrated high precision in predicting the aqueous solubility and stability of active pharmaceutical ingredients (APIs) (8).

### **1.2.AI-Driven Excipient Selection and Enhancement**

A critical element in effective pharmaceutical formulations involves choosing and refining excipients, which profoundly influence patient compliance, drug stability, bioavailability, and production viability. high-dimensional datasets can be processed via AI, particularly ML methods (Mol2vec combined with molecular features + stacking ensembles), delivering strong performance (AUC 0.93). This uncovers concealed patterns and nonlinear dependencies governing excipient efficacy. Across diverse processing and environmental conditions, these models predict excipient-API interactions and those with other formulation components. Such forecasting capabilities can accelerate robust formulation development and substantially reduce reliance on extensive wet-lab experiments (9).

### **1.3. Predictive Analytics for Formulation Optimization**

Machine learning algorithms such as random forests (RF), support vector machines (SVMs), artificial neural networks (ANNs), and genetic algorithms (GAs) have been widely applied to optimize pharmaceutical formulations. These approaches process large datasets to uncover complex nonlinear correlations between formulation variables (e.g., excipient selection and

levels, manufacturing parameters) and performance metrics (e.g., stability, bioavailability, dissolution kinetics), which conventional methods often fail to detect (10).

Support vector machines (SVMs), another machine learning approach, excel in both regression and classification applications. Their ability to construct decision boundaries in multidimensional spaces makes them effective for distinguishing favorable from suboptimal formulation parameters. In nanoparticle optimization research, SVMs demonstrated superior performance over regression models for forecasting particle size and zeta potential (11).

Genetic algorithms (Gas), alongside predictive modeling, serve as powerful optimization tools. These evolution-inspired methods iteratively evolve toward optimal formulation parameters through simulated natural selection. Gas are commonly paired with ANNs or other ML frameworks to build integrated systems capable of both forecasting and refining formulation performance (12).

**Table 1: AI Techniques in pharmaceutical review and optimization process**

<b>AI models</b>	<b>Advanced description for review process</b>
Genetic Algorithm (GA)	Evolutionary optimization algorithms grounded in the principle of natural selection and genetic inheritance, extensively employed to systematically refine formulation composition, optimize drug release characteristics and fine tune critical targeted dosage form performance (13).
Artificial Neural Network (ANN)	Data-driven computational models capable of capturing complex, non linear relationship among formulation variables, processing conditions and drug release kinetics, thereby enabling predictive evaluation and optimization of pharmaceutical formulation during the review phase (14).
Support Vector Machine (SVM)	Supervised machine learning models utilized to establish high accuracy predictive relationship between excipient composition, processing parameters and resultant drug release profiles, contributing to robust formulation design space assessment (15).
Particle Swarm Optimization (PSO)	A population based metaheuristic optimization approach inspired by collective swarm behavior applied to enhance formulation attributes such as particle size distribution, dissolution efficiency and overall dosage form (16).
AI based Expert System	Knowledge driven system integrating rule based reasoning and fuzzy logic to stimulate expert decision making, supporting systematic evaluation and optimization of dosage form variables during regulatory and formulation review processes (17).
Monte Carlo Simulation	Probabilistic simulation techniques employed to asses uncertainty and variability in formulation and manufacturing parameters, facilitating risk based decision making and development of robust pharmaceutical product (18).
Computational Fluid Dynamics (CFD)	Advanced numerical modeling tools used to analyze fluid flow, mixing dynamics and mass transfer phenomena in unit operations such as granulation, coating and drying, aiding in process understanding and optimization (19).
Response Surface Methodology (RSM)	Statistical modeling and optimization methodology used to quantify interactions among multiple formulation and process variables, enabling efficient identification of optimal conditions and performance response (20).

## 2. AI in drug discovery

Developing novel drugs through research and development remains a daunting, costly, and protracted endeavor. Typically, the R&D timeline stretches 10–15 years. Even with substantial investments from the pharmaceutical sector, the quest for the next major therapeutic breakthrough endures (21). AI methodologies and platforms excel at swiftly pinpointing hit and lead compounds, confirming drug targets, and refining molecular architectures, ultimately aiding the healthcare sector by shortening discovery timelines and curbing costs for new chemical entities (22).

QSAR-based computational models enable rapid prediction of vast compound libraries or specific physicochemical properties, such as logP or logD values (23). Deep learning models surpass conventional machine learning approaches across 15 drug candidate ADMET datasets in terms of predictive accuracy. AI tools such as XenoSite, FAME, and SMARTCyp effectively pinpoint drug metabolism sites (24).

**Table 2: AI Platforms in Drug Design**

<b>Name of tools</b>	<b>Application</b>
Reinforcement learning	Used to optimize drug combination and dosages by considering multiple interacting variables and maximizing desired outcome.
DeepChem	Open source library for deep learning in chemistry and drug discovery.
DeepTox	Open source deep learning framework specifically designed for toxicity prediction and assessment.
Natural graph fingerprints	Method for encoding molecular structure as fixed length feature vector using neural network, suitable for various application in drug discovery such as virtual screening, lead optimization and property prediction.
PotentialNet	Ligand binding affinity prediction based on graph convolutional neural network (CNN).
Predictive ADME / Tox modeling	Tools employ ML techniques to model and predict the absorption, distribution, metabolism and excretion and potential toxicity of drug candidates.
Natural language processing (NLP)	Assist in extracting and analysing information from scientific literature, patents and clinical trial data.
Cheminformatics	Tools enable the analysis and manipulation of chemical structure and properties.
QSAR/ QSPR	Correlate molecular properties and structure with biological activities or properties enabling the prediction of compound behaviour.
Deep learning (DL)	Applied in tasks like virtual screening, de novo drug design and predicting drug properties.
Machine learning (ML)	Help predict drug target interactions, analyse biological activity and optimize lead compound.

### **3.AI in drug development**

QSPR-based computational approaches can tackle key formulation challenges like stability deficits, solubility hurdles, porosity variations, and beyond (25). Piroxicam direct-fill hard gelatin capsules were formulated via a combined approach integrating expert systems (ES) and artificial neural networks (ANN) to attain the target dissolution characteristics. The Model Expert System (MES) provides decisions and guidance for recipe optimization using input variables. In contrast, ANN employs backpropagation training to correlate formulation inputs with performance outputs, facilitating seamless recipe design. A central control unit coordinates the workflow (26).

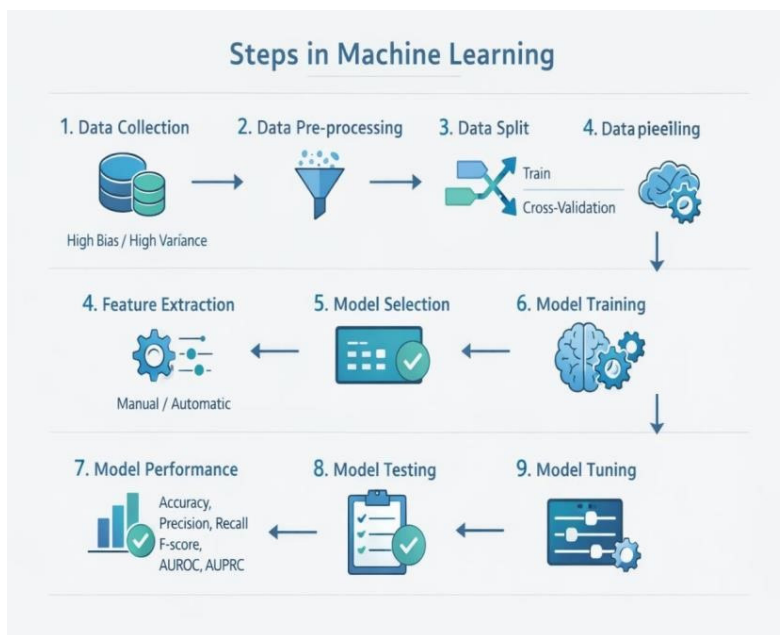
Researchers have employed diverse computational approaches such as computational fluid dynamics (CFD), discrete element modeling (DEM), and finite element analysis (FEM) to examine how powder flow characteristics influence die-filling and tablet compaction processes (27) CFD can additionally assess the impact of tablet geometry on disintegration behavior (28). AI applications in pharmaceuticals also encompass drug repurposing (29), pharmacological profiling (30), protein properties and potency (31), combination therapies, drug-target binding (32) and forecasting synthetic routes for drug-like entities (33). Furthermore, linking drugs to diseases, plus discovering new biomarkers and therapeutic targets via omics data analysis, reveals novel pathways and objectives (34).

### **4.AI driven computational strategies in modern drug discovery**

#### **4.1.Machine learning approaches in drug discovery**

AI driven computational strategies have become integral to modern drug discovery by accelerating target identification, molecular design and clinical decision making. Machine learning used in this field are broadly classified into supervised and unsupervised methods (35).Supervised learning relies on labeled dataset to predict efficacy, safety, target interactions and adverse drug reactions. In contrast unsupervised learning analyses unlabelled data to uncover hidden patterns, identify novel therapeutic targets and classify chemical entities based on shared structural and physicochemical properties.

Commonly employed algorithm such as random forest which are capable of efficiently managing high dimensional feature spaces, support vector machine which demonstrate strong performance in classification tasks through the construction of optimal separating hyper planes (36), and gradient boosting techniques which sequentially combine multiple weak predictive models to generate highly accurate and robust learners (37). Collectively, these machine learning methodologies contribute to the acceleration of the drug discovery pipeline by enabling efficient large scale data interrogation and facilitating the prioritization of promising drug candidates (38).



**Fig 1: Steps in Machine learning**

#### 4.2. Deep neural network

Deep neural network, particularly convolutional neural network (CNN) and recurrent neural network (RNN), have emerged as highly potent methodologies in contemporary drug design. CNN demonstrate exceptional proficiency in handling image-analogues molecular data, including chemical structure encoded as two-dimensional representations or three-dimensional point cloud models. These networks possess the capacity to autonomously extract hierarchical features, thereby capturing intricate spatial and structural patterns that are critical for molecular characterization and predictive modeling in drug discovery (39). These architectures have been successfully employed to forecast protein-protein interactions, characterize drug metabolizing enzyme behavior and computational generate novel drug like chemical entities (40).

#### 4.3. Artificial neural network

ANNs consist of multiple interconnected functional units designed to emulate the transmission of electrical impulses within the human brain, thereby mimicking biological cognitive processes. These system are predominantly inspired by biological neural architectures. ANNs process input data and autonomously learn from it, fundamentally, artificial neurons perform weighted summation of incoming signals and generate corresponding outputs (41).

#### 4.4. Graph neural network

GNN employ an iterative message passing or neighbourhood aggregation framework through which each node assimilate feature information from its adjacent nodes, progressively refining its latent representation. This process enables the simultaneous learning of both localized interactions and global topological pattern embedded within

the graph. Prominent GNN architecture encompass Graph Convolutional Network (GCNs), which leverage spectral or spatial convolutional, Graph Attention Network (GATs) which incorporate attention mechanism to differentially weight the influence of neighbouring nodes, and GraphSAGE which facilitates scalable, inductive representation learning suitable for large scale graphs (42).

#### **4.5. Deep learning**

Deep learning methodologies are increasingly leveraged for silico toxicity assessment. By interrogating extensive chemical datasets alongside their corresponding toxicity annotations, these models can uncover latent structure-toxicity relationship that may elude conventional expert analysis. This capability support the early-stage identification of potentially hazardous compounds thereby mitigating the likelihood of adverse outcome during clinical evaluation and significantly enhancing overall drug safety (43).

#### **4.6. Natural language processing**

Natural language processing (NLP) analyses large amount of unstructured text from scientific literature, patent and electronic health records to identify novel drug targets and therapeutic candidates, supporting innovative drug discovery and development. Furthermore, patent focused NLP analyses support the discovery of previously unreported chemical entities, provide insights into intellectual property landscape, and assist in identifying prospective collaborators or licensing opportunities (44). Transformer based models (e.g BERT, GPT, T5) outperform RNNs by enabling parallel processing and improved performance in tasks like translation and text synthesis, driving advance in computational biology and protein language models (45).

#### **4.8. Fuzzy logic**

Fuzzy logic represents a predominant computational paradigm with artificial intelligence and is extensively employed for sophisticated problem-solving application. When integrated with artificial neural network (ANNs), it facilitates enhanced comprehension of system formulation and optimization mechanism.

#### **4.9. Molecular Fingerprinting**

Molecular fingerprinting refers to a computational methodology that encodes chemical entities into condensed numerical descriptors, such as binary vector or multidimensional feature matrices, enabling the abstraction of essential structural and physicochemical attributes. These descriptors support high throughput similarity assessment, molecular comparison and machine learning driven analyses, thereby playing a pivotal role in contemporary drug discovery and materials science. Widely adopted fingerprinting schemes include circular representations such as extended connectivity fingerprints (ECFP) for sub structural characterization, path based fingerprint that capture bond connectivity sequences and three dimensional fingerprint designed to represent molecular conformations and spatial geometry (46). Advanced computational platform such as RDKit (47) and ChemDes (48) are extensively employed for the high throughput generation of molecular fingerprint, thereby serving as an effective interface that integrates chemical informatics with artificial intelligence driven methodologies (49).

#### **4.10. Reinforcement learning and evolutionary algorithm**

Reinforcement learning (RL) presents a robust method for drug refinement by modeling it as a sequential decision task. Here, an agent (the RL model) learns to select actions (e.g., altering molecular architecture or tuning dosage) to optimize a reward function, like therapeutic potency, while reducing adverse effects. RL methods can navigate the expansive realm of potential drug entities and dosing protocols, uncovering superior candidates that might elude conventional human analysis (50).

Evolutionary algorithms, drawing from Darwinian principles, offer an effective strategy for refining molecular architectures. These techniques emulate biological evolution—through processes like variation and culling—to iteratively evolve and enhance molecular designs meeting target attributes. By progressively tweaking molecular scaffolds and assessing their suitability against specified metrics (e.g., ligand affinity and drug-likeness), evolutionary algorithms adeptly traverse chemical space to unveil innovative therapeutic leads with superior characteristics (51).

#### **4.11. Generative AI**

Generative AI platforms like ChatGPT offer substantial promise in medical training and patient management. Within pharmacy, they can boost productivity by supporting prescription evaluations, medication interaction assessments, and side-effect surveillance, thereby elevating care quality. Yet, their integration into pharmacy curricula is largely uncharted, with scant studies addressing deployment hurdles, highlighting the imperative for deeper exploration (52).

### **5. Application of AI in drug discovery**

#### **5.1. Target identification and validation**

Artificial intelligence (AI) has emerged as a transformative paradigm in drug discovery, substantially enhancing the accuracy and throughput of target identification and validation processes. By enabling the integrative analysis of diverse and high dimensional biological datasets – including genomics, proteomics, and other multi-omics platform – AI based computational framework surpass the limitations of traditional target discovery methodologies (53). These advanced algorithms facilitate the systematic identification of novel and disease relevant molecular targets through the extraction of latent and complex biological relationship (54).

#### **5.2. Drug screening and lead discovery**

AI driven virtual screening and in silico methodologies have profoundly transformed contemporary drug discovery paradigms by enabling the rapid identification of high value lead molecules (55). Machine learning (ML) algorithm constitute a central component of these strategies; for example, quantitative structure- activity relationship (QSAR) models are constructed to establish predictive correlations between molecular architecture and biological efficacy (56). Such models facilitate the systematic screening

of vast compound repositories and enable the prioritization of candidate exhibiting the greatest likelihood of effective target engagement (57).

### **5.3. Drug optimization and design**

AI enabled methodologies are fundamentally transforming drug optimization and molecular design by enhancing the precision with which key physicochemical and biopharmaceutical attributes such as solubility, stability, and bioavailability are optimized (58). Machine learning algorithms are capable of interrogating large scale chemical datasets to elucidate structure property relationship and accurately predict critical parameters (59).

For instance, quantitative structure activity relationship (QSAR) modeling typically relies on datasets comprising approximately 1,000-5,000 compounds to achieve robust predictive performance (60). In protein function prediction, investigators integrate curated data from publicly accessible repositories such as UniProt Consortium (61) and the Protein Data Bank (PDB) which provide extensive protein sequence and structural information across multiple species (62).

### **5.4. Preclinical and clinical development**

Machine learning algorithms are capable of interrogating extensive repositories of chemical structural data along with their corresponding pharmacokinetic and pharmacodynamic attributes to forecast critical parameters such as absorption, distribution, metabolism and excretion (ADME) as well as potential drug – drug interactions. Deep learning framework in particular can precisely estimate drug permeability across biological membrane, whereas complementary computational models can emulate in vivo distribution patterns (63).

## **6. Recent Advances in Pharmaceutical Drug Delivery Technologies**

### **6.1. Controlled release tablet formulation**

Researchers use computer simulations of how drugs move through the body (pharmacokinetics) and artificial neural networks (ANN) to create slow-release drug tablets (64). The ANN learns complex patterns from input and output data using Chem software. To predict the best tablet recipes, scientists train a smart ANN model on two ideal lab dissolution curves and two target body release curves. In the body, drug dissolution is the slowest step that controls absorption, as it directly matches the amount of drug absorbed. Lab release patterns are compared using difference (f1) and similarity (f2) scores (65).

### **6.2. Immediate release tablet formulation:**

To improve tablet durability, Turkoglu created a direct-compression formula for hydrochlorothiazide tablets (66). In another study, Kesavan and Peck built a model for caffeine tablets that explained the amounts of fillers and binders, processing steps (like granulator type and binder addition method), and tablet qualities (disintegration time, hardness, and friability). These studies showed neural networks outperformed traditional

stats methods. Academics later re-tested Kesavan and Peck's results with genetic algorithms and neural networks (67). The work highlighted how the importance of output traits and limits on ingredients/processing steps shaped the best formula (68).

### **6.3. Hard gelatin capsule shell formulation:**

Creating hard gelatin capsule formulas relies on smart tools like artificial neural networks (ANN) and expert systems (ES). ANNs mimic human brain functions such as learning, predicting, generalizing, and pulling insights from specific knowledge. They quickly turn lab data and stats into useful knowledge, helping manufacturers create targeted strategies for future batches or predict formula properties. In 2005, Wendy I. Wilson expanded the Expert Network and analyzed capsule shells for Biopharmaceutical Classification System (BCS) Class II drugs like carbamazepine, ketoprofen, naproxen, and ibuprofen.

Capsugel's expert system for powder-in-capsule formulas was used worldwide, though it only suggested compositions and had limits. Early tests showed poor prediction accuracy and high errors. After retraining the ANN with fresh data, models reached an  $R^2$  under 70%. For the drugs, the smart hybrid system predicted about 5% drug solubility. Using just 10% of new data for validation, researchers proved it could design formulas meeting performance goals. They showed its power for various BCS Class II drugs by factoring in wettability and dissolving traits(69).

### **6.4. Solid dispersion(SD):**

Solid dispersions are one or more active drug ingredients (APIs) spread evenly in a solid carrier material (70). They're a practical, low-cost way to boost drug solubility and absorption in the body (71). Many AI-driven solid dispersion studies apply artificial neural networks (ANNs) to fine-tune formulas (72). Researchers used artificial neural networks (ANNs) to explain links between factors like API amount, PEG's molecular weight, and temperature in an SD with PVP. Recently, they built a machine learning (ML) model to predict SD stability. It used 20 molecular features to compare 8 ML methods. The random forest (RF) model was most accurate and revealed each input's role. The top 5 key factors from the 20 were: drug loading ratio, room humidity, storage temperature, preparation temperature, and polymer molecular weight (73).

### **6.5. Emulsion, Microemulsion and Nanoemulsion**

Emulsions are two-phase mixtures where water and oil are spread together and held stable by an emulsifier (74). Using micro- and nanoemulsions offers benefits like better drug absorption (API bioavailability), clear appearance, and longer stability (75).

**Table 3: AI – Enabled Software Platform for the Development and Optimization of Liquid Dosage Forms**

<b>Software Platform</b>	<b>Core Capabilities</b>	<b>Functional</b>	<b>AI/ML Integration</b>	<b>Application in Liquid Dosage Formulation</b>
QbD works	Comprehensive Quality Design (QbD) framework supporting pharmaceutical formulation design and process development	by	Employs Machine Learning algorithm for risk assessment, multivariate process optimization and predictive analysis	Facilitates prediction and optimization of critical attributes such as formulation stability, rheological behavior(viscosity) and dissolution performance (76).
SimSci PRO/II	Advanced simulation tailored for chemical and pharmaceutical manufacturing operations	process software	Integrates AI supported algorithm for real time process optimization and adaptive control strategies	Enables virtual simulation and optimization of heating, cooling and mixing operations involved in liquid formulation manufacturing (77).
Zoom Lab	AI driven digital platforms specifically developed for pharmaceutical formulation research	digital	Utilizes artificial intelligence throughput formulation screening predictive modeling	Assists in identifying optimal excipient systems and elucidating drug solvent and excipient interaction mechanism on liquid formulation (78).
Aspen Plus	Robust modelling and optimization software widely used in pharmaceutical scale up studies	process and software	Incorporate AI assisted simulation tools to enhance process efficiency and stability	Supports optimization of component ratios and facilitates scale up strategies for liquid dosage form production (79).
SuperPro Designer	Integrated platform for process modelling, techno economic analysis and cost estimation	platform	Applies AI based decision support tools to evaluate alternative production pathways and resource utilization	Employed in batch process design, cost optimization and scale up of liquid dosage formulation (80).

PAT Solut ion	Process Technology systems with advanced monitoring capabilities	Analytical (PAT) embedded	Leverages AI for real time quality surveillance, anomaly detection and predictive maintenance	Ensures continuous monitoring of Quality (CQAs) during liquid dosage form manufacturing (81).
LabD CT	Digital platform laboratory industrial simulation	twin based for scale and process	Uses AI powdered virtual modelling to replicate real world production condition	Enables in silico testing and optimization of liquid formulation within simulated manufacturing environment (82).

**Table 4: AI tools in parenteral formulation**

AI tools / techniques	Types of mode	Application in parenteral formulation	Benefits
Artificial Neural Network (ANN)	Deep Learning	Optimization of drug concentration, excipient ratio, pH	Reduces trial and error experiments
Machine Learning Learning (Random Forest, SVM, Gradient Boosting)	Supervised Learning	Stability prediction & shelf-life estimation	Improves prediction accuracy
AI-integrated Design of Experiments (DoE)	Optimization Model	Selection of Critical Process Parameters (CPP)	Supports QbD approach
QSAR Modeling	Predictive Modeling	Prediction of solubility, permeability, toxicity	Early-stage screening of injectable drugs
Molecular Docking (AutoDock, Schrödinger)	Computational Simulation	Drug–excipient compatibility studies	Reduces incompatibility issues
AI-based Image Analysis	Computer Vision	Particle size & particulate matter detection	Ensures sterility & pharmacopeial compliance
Predictive Analytics	Data-driven Modeling	Risk assessment & batch failure prediction	Enhances quality control
Digital Twin Technology	Process Simulation	Virtual modeling of sterile manufacturing	Better scale-up & real-time monitoring
MATLAB / Python AI Models	Data Analytics	Drug release kinetics modeling	Accurate release prediction
Bayesian optimization	Statistical AI Model	Formulation variable optimization	Saves time and resources

## 6.6.AI for Nanomedicine

AI revolutionizes nanomedicine through data analysis, pattern recognition, and optimization, accelerating nanoscale interventions, diagnostics, targeted delivery, and personalized therapies (83).

- Nanoparticle Design: AI predicts physicochemical properties, stability, and efficacy for tailored nanoparticles in imaging, sensing, and synergistic cancer drug delivery (e.g., deep learning for melanoma diagnostics)
- Biological Modeling: AI simulates nanoscale interactions, drug release kinetics, toxicity, and nanosensor monitoring of biomarkers for real-time, personalized interventions (84).
- Scale-Up and Optimization: AI automates nanocarrier databases, evaluates drug loading/stability/retention, and uses Monte Carlo/molecular dynamics for 3D structure property predictions, reducing experiments (85).

## 6.7.AI for 3 – D printed dosage form

AI transforms 3D-printed dosage forms, enabling personalized medicine via patient-specific optimization (e.g., age, weight, history). ML analyzes datasets to simulate drug release, dosage, geometries; predicts manufacturing issues; and refines printing parameters (nozzle/platform temperature, speed) for quality, reproducibility, and scalability (86). Techniques include fused-filament fabrication, binder jetting, laser sintering, and microsyringe extrusion. Example: Obeid et al. used ANN modeling and self-organizing maps to optimize diazepam 3D-printed tablets, linking infill pattern/density, surface area/volume to enhanced dissolution—validated experimentally (87).

## 7.Contemporary Applications of Artificial Intelligence in the Pharmaceutical Industry

AI is revolutionizing pharmaceutical manufacturing and drug development by optimizing excipient selection, synthesis routes, process design, supply chains, and maintenance—saving time and costs across stages (88).

- Drug discovery: Cuts 3–6 year timeline by 1–2 years via faster hit identification, lead optimization, and preclinical predictions of efficacy/toxicity; reduces costs (35% of \$2.8B total) by fewer tests and higher early-trial success (89).
- Clinical trials: Optimizes designs, recruitment, monitoring, and dosing; shortens trials 15–30%; boosts Phase 1 success to 80–90% (vs. 40–65% historical), Phase 2 to ~40%; could raise overall success from 5–10% to 9–18% (90).

### 7.1. Target Identification

AI speeds target discovery using vast genomic data (e.g., AstraZeneca's 2M sequences by 2026) to pinpoint disease-causing variants, genes, and pathways. Integrates with

CRISPR screens via ML/DL for analyzing image outputs, identifying genes linked to cancer drug resistance/sensitization (91).

## 7.2. Drug Design

Post-target ID, AI predicts molecular structures/properties from biological datasets to design optimal candidates. Insilico Medicine screened billions of molecules, developing an idiopathic pulmonary fibrosis drug in 18 months, advancing to preclinical trials (92).

## 7.3. Compound Selection

AI screens chemical libraries for high-potential candidates based on solubility, permeability, toxicity, and physicochemical properties. Exscientia designed EXS4318 (PKC- $\theta$  inhibitor for autoimmune diseases) in 11 months (150th molecule), with superior potency/selectivity; licensed by Bristol Myers Squibb in 2023 (93).

## 7.4. Synthesis Route

Prediction AI streamlines retrosynthesis, a tedious process, via tools like IBM's RXN for Chemistry—a deep learning model trained on 2.5M reactions using molecular transformers to predict outcomes, pathways, and procedures by correlating chemical motifs (94).

### 7.4.1. Single-Step Retrosynthesis Challenges

Reaction center ID: Mimics chemist's bond-breaking decisions; tough due to multiple pathways, requiring generalization beyond rules (95). Reactant/reagents generation: Ensures validity via (i) chemically correct molecules, (ii) feasible reactions (selectivity, conditions, effects), (iii) atom conservation. Graph methods suit molecular graphs; sequence-based fit SMILES (96).

### 7.4.2. Multi-Step Retrosynthesis Challenges

Exponential search space, ambiguous "good route" criteria (e.g., cost/stability in industry vs. novelty in academia), limited datasets. AI accelerates discovery and automates evaluation across contexts (97).

## 7.5. Robotic Synthesis

AI-integrated robotics automate high-throughput synthesis, executing reactions, real-time monitoring, and parameter adjustments. University of Glasgow's Chemputer speeds smallmolecule drug synthesis (98).

## 7.6. Process Optimization

AI analyzes production data to fix inefficiencies, optimize conditions, and scale up. Pfizer used AI for COVID-19 vaccine yield improvement, production speedup, temperature prediction in 3000+ freezers, and lipid nanoparticle simulations to minimize allergies (99).

### **7.7. Continuous Manufacturing & PAT**

AI enhances continuous flow (vs. batch) via real-time probes (Raman/NIR) for parameter monitoring/adjustments, boosting efficiency from raw materials to packaging (100).

### **7.8. Digital Twin Technology**

AI creates virtual process replicas for simulation/optimization without downtime. Johnson & Johnson uses them to replicate/test manufacturing across sites, accelerating market speed (101).

### **7.9. Predictive Maintenance**

AI analyzes sensor data to forecast equipment failures, enabling proactive scheduling. Reduces downtime/costs; implemented by Pfizer and others (102).

### **7.10. Supply Chain Optimization**

AI forecasts demand, manages inventory, and streamlines logistics via ML on market/performance data. Novartis' Buying Engine centralizes procurement (lab supplies, PPE, parts) using knowledge graphs, recommenders, optimization, and ML for real-time transparency and efficiency, cutting costs (103).

### **7.11. Medical Imaging**

Bayer employs NLP (like GPT) for medical coding, translating physician reports to standardized terms with 96% accuracy (millions processed since 2017). Calantic Digital Solutions (with Blackford Analysis) automates radiology tasks, speeds workflows, reduces workload, and improves detection for faster patient decisions (104).

## **Conclusion**

Artificial Intelligence is fundamentally revolutionizing the pharmaceutical industry by optimizing every stage of the drug life cycle, from preformulation and molecular design to manufacturing and supply chain management. By integrating advanced computational models, the industry can achieve higher predictive precision, reduce reliance on labor-intensive wetlab experiments, and significantly shorten the time-to-market for new therapeutics. AI-driven strategies, such as predictive analytics for formulation optimization and robotic synthesis, are proving essential in overcoming traditional challenges like solubility hurdles and stability deficits. Ultimately, the continued integration of AI promises a more efficient, cost-effective, and personalized approach to drug development and healthcare delivery.

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### **Conflict of interest**

The authors declare no conflict of interest.

### **Data Availability**

No new data were created or analyzed in this study.

### **Author Contribution**

**Gopika K-** Conceptualization, Methodology, Writing-original draft, Writing-review and editing.

**S. Enamul Hasan** - Conceptualization, Methodology, Writing-original draft, Writing-review and editing.

**G. Alagumanivasagam** - Project administration, supervision, Writing-review and editing.

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