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Review Article

Artificial Intelligence (AI)'S Transformative Impact on Drug Development and Regulatory Affairs: A 2025 Review

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Abstract

Artificial Intelligence (AI) is revolutionizing the pharmaceutical industry by accelerating drug discovery, enhancing the efficiency of clinical trials, and enabling the development of personalized medicine. It is also being used in pharmaceutical regulatory affairs to automate the regulatory filling and document management. This review highlights the current applications of AI in drug development and pharmaceutical regulatory affairs, explores key case studies and technological advancements, and discusses the challenges and regulatory considerations associated with these applications. As the AI drug discovery market is growing significantly [1], understanding its integration within pharmaceutical pipelines is critical for stakeholders across industry and academia.

Keywords: Artificial Intelligence, Drug Discovery, Machine Learning, Clinical Trials, Personalized Medicine, Drug Repurposing, Predictive Analytics, Regulatory Frameworks, Generative AI, Pharma Innovation

Abbreviations: AI: Artificial Intelligence; FDA: Food and Drug Administration; NLP: Natural Language Processing; SaMD: Software as a Medical Device.

Introduction

Pharmaceutical industry plays a critical role to address healthcare challenges and respond to medical emergencies which is mainly based on continuous innovation and application of new technologies. The core steps of pharmaceuticals innovation include extensive research and development, manufacturing process development and optimization, packaging considerations, and patient oriented marketing strategies [2].

The traditional drug development process is time-consuming, costly, and fraught with high failure rates. The challenges are even more extensive during the development of novel therapeutics and

complex manufacturing process. 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 safety, quality and efficacy [3]. AI offers promising solutions by expediting various phases of drug development, from target identification to clinical trials. In 2025, the market for AI in drug discovery is valued at approximately $1.94 billion and is expected to reach $16.49 billion by 2034. This growth underscores AI's transformative potential in modernizing pharmaceutical R&D.

AI can be implemented to simplify the regulatory affairs activities like- dossier compilation, documents archiving and review, data extraction, compliance auditing and quality management system. This human AI- Human interaction opens new era in pharmaceutical regulatory affairs [4]. The European Medicines Agency (EMA) and Food and Drug Administration (FDA) have plans to implement AI and are currently consulting stakeholders for their comments.

Materials and Methods

This review was conducted through an extensive literature analysis of peer-reviewed journals, company reports, regulatory documents, and market studies published between 2017 and 2025. Key search terms included "AI in drug discovery," "machine learning in pharma," "generative AI for molecules," and "regulatory AI in medicine." Data from PubMed, Scopus, and Google Scholar formed the basis of this synthesis.

Results and Discussion

AI in the Life Cycle Management of Pharmaceuticals

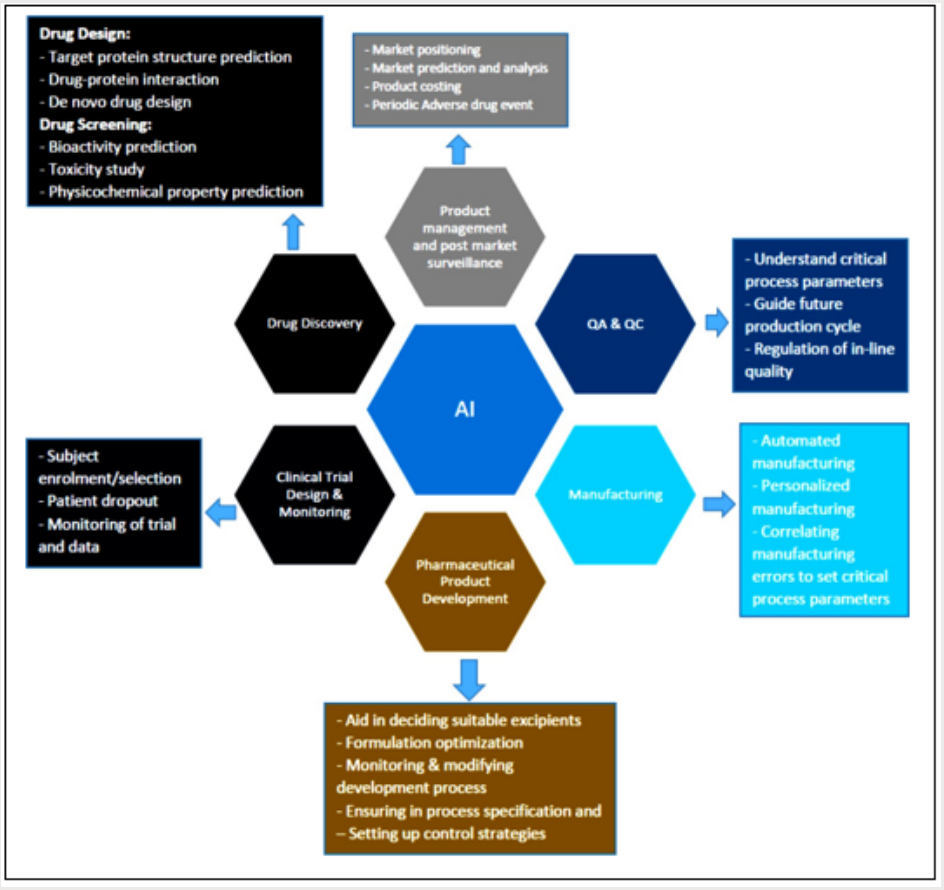

Figure 1: AI in various pharmaceutical business subclass, including pharmaceutical product management and drug development [5].

Table 1

Name of tools/techniques	Application
DeepChem	Open-source library for deep learning in chemistry and drug discovery
Reinforcement learning	Used to optimize drug combinations and dosages by considering multiple interacting variables and maximizing desired outcomes
Neural graph fingerprints	Method for encoding molecular structures as fixed-length feature vectors using neural networks, suitable for various applications in drug discovery, such as virtual screening, lead optimization, and property prediction
DeepTox	Open-source deep learning framework specifically designed for toxicity prediction and assessment
Predictive ADME/Tox modelling	Tools employ ML techniques to model and predict the absorption, distribution, metabolism, excretion, and potential toxicity of drug candidates
Natural language processing (NLP) tools	Assist in extracting and analysing information from scientific literature, patents, and clinical trial data
Cheminformatics tools	Tools enable the analysis and manipulation of chemical structures and properties
QSAR/QSPR modelling	Correlate molecular properties and structures 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 compounds

AI can support different stages of drug research and development and throughout the life cycle of the pharmaceuticals. AI can actually be implemented from the lab to the bed. Main steps are Drug discovery, Clinical trial design & monitoring, Pharmaceuticals product development, Manufacturing, Quality control & assurance, Product management and post market surveillance. A number of AI tools/technique which are widely use now in the pharmaceuticals industry is tabulated below [5] (Table 1) (Figure 1).

AI's Role in Modern Drug Formulation

The pharmaceutical industry is increasingly turning to artificial intelligence (AI) to solve complex problems in drug formulation. Traditional dosage forms are being enhanced—or replaced—by more advanced systems like nanoemulsions, capsules, and solid dispersions, thanks in large part to machine learning and neural network models. These technologies help scientists overcome typical formulation barriers such as poor solubility, inadequate stability, and inconsistent bioavailability [6].

Controlled Release Dosage form

To develop tablets that release drugs gradually over time, researchers use AI-based tools to simulate how medications behave in the body. Artificial Neural Networks (ANNs), in particular, have proven effective in

fine-tuning how quickly a drug dissolves and is absorbed, helping to align lab-based release profiles with real- life performance [7].

Fast-Acting Tablets

When immediate effects are needed, AI again plays a key role. Rather than relying solely on trial and error, formulators use neural networks and optimization algorithms to evaluate the right mix of ingredients and manufacturing processes [8]. These approaches provide more reliable results than traditional statistical models.

Capsule Formulation

Hard gelatin capsules—often used for drugs with poor water solubility—also benefit from AI. These systems mimic human reasoning to predict how different ingredients will interact. Though early versions struggled with accuracy, refinements in machine learning have led to much better predictive models, especially when working with data from similar drug types [9].

Solid Dispersions

AI is widely used in improving formulations where the active drug is embedded in a solid base. These systems are known for enhancing solubility and stability. Using techniques like random forest models, scientists can now identify which factors—such as polymer choice or humidity levels—most influence final product quality.

Emulsions and Nanoemulsions

These complex mixtures of oil and water are stabilized with emulsifiers and require careful formulation. AI tools assist in adjusting ingredients to achieve the right balance of particle size, texture, and shelf-life [10]. In some cases, neural networks can even predict product performance based on thermal and structural data.

Self-Emulsifying Systems (SEDDS)

SEDDS are designed to help drugs dissolve in the body more effectively. AI is used here to model how the formulation behaves during digestion, ensuring optimal absorption. Researchers apply advanced algorithms to determine the right blend of oils, surfactants, and drugs, tailoring each formulation to meet specific bioavailability needs.

Other Applications

Beyond these examples, AI continues to be integrated into the creation of microparticles [11-15], nanoparticles [16-29], liposomes [30], microspheres [31-33], and various solid and liquid drug forms. Its ability to process complex data quickly makes it an invaluable tool for modern pharmaceutical development.

AI's Role in Pharmaceutical Regulatory Affairs

Traditional Approach

The manual process of regulatory affairs involves:

i. Data collection and dossier preparation, which is time-consuming, prone to manual errors, and results in a heavy workload.

ii. Document review and dossier submission are also labor-intensive and inefficient.

AI-Driven Regulatory Affairs

With AI implementation, the process is transformed, offering [34]:

a) Easy documentation and submissions

b) Real-time monitoring and seamless data exchange

c) Enhanced regulatory intelligence

d) Improved decision-making and compliance

e) Optimization of workflows

f) Risk assessment and predictive modeling

g) Faster approval with a higher success rate

Overall, AI streamlines and enhances the efficiency, accuracy, and speed of regulatory processes in pharmaceutical and healthcare sectors.

Conclusion

AI is driving a paradigm shift in drug development, offering solutions to overcome long-standing pharmaceutical R&D challenges. Addressing integration barriers, regulatory clarity, and ethical use will ensure its sustained impact. The use of AI in pharmaceutical formulations is predictable and will continue to be transformative. AI aids researchers in identifying new drug targets, drug interactions, and patient populations that can most benefit from treatment. With increasingly advanced AI systems, researchers can accurately simulate biological systems and develop more personalized treatments, leading to more efficient and targeted drug development. In the fast-paced and rapidly changing environment of pharmaceutical regulatory affairs, the ability to apply AI to the many tasks involved is a major step up. That includes not only more time-efficient regulatory dossier creation, but also better processes for risk analysis and other key regulatory aspects.

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Conflict of Interest

The authors declare no conflict of interest.

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