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Exploring the world of AI- The impact in pharmaceutical science

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Abstract

Artificial Intelligence (AI) has emerged as a transformative force in the pharmaceutical industry, addressing the long-standing challenges of high costs, lengthy timelines, and high attrition rates in drug development. From early expert systems like DENDRAL and MYCIN to advanced deep learning models such as AlphaFold and AtomNet, AI has progressively reshaped every stage of the drug development pipeline. Its applications range from target identification, de novo molecule design, and clinical trial optimization to manufacturing and pharmacovigilance. This paper traces the historical evolution of AI in pharmaceuticals, highlights key milestones, and explores the growing necessity of AI software in modern drug discovery and healthcare innovation.

Keywords: Deep Generative Model; Drug Repurposing; Design Make Test Learn Cycle [DMLT]; Human Genome; Personalized Medicine; Protein and Docking Study

1. Introduction

Drug discovery and development are traditionally complex, costly, and time-consuming processes, often taking more than a decade and billions of dollars to bring a single therapy to market. The high rate of late-stage failures further amplifies the need for more efficient and predictive approaches. In this context, Artificial Intelligence (AI) has emerged as a revolutionary tool, capable of analyzing massive datasets, learning hidden patterns, and generating actionable insights beyond conventional methods.

The role of AI in pharmaceuticals has evolved significantly from rule-based expert systems in the 1970s to advanced machine learning and generative models in the 21st century. These technologies now support a wide range of applications, including computational chemistry, drug repurposing, personalized medicine, and smart manufacturing. Tracing this historical trajectory provides a comprehensive understanding of how AI has transitioned from experimental computational tools to an indispensable component of pharmaceutical innovation.

2. Emergence of Artificial Intelligence

The emergence of Artificial Intelligence (AI) as a formal discipline in the mid-20th century was the culmination of centuries of philosophical thought and decades of rapid advancement in computer science. Unlike a single invention, AI emerged from a convergence of ideas across multiple fields, marking a pivotal moment in the quest to create thinking machines.

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2.1. Key Stages in AI Development

2.1.1. 1950- Turing Test (Imitation game)

Introduced a practical behavioural criterion for machine intelligence and set the philosophical framework for AI research [1].

2.1.2. 1956 -Dartmouth Summer Research Project on Artificial Intelligence

The field is formally founded and researchers establish core goals like symbolic reasoning, problem solving, learning [2].

2.1.3. 1966 -ELIZA (Early Natural-Language Program)

Demonstrated how simple pattern-matching can mimic conversation and revealed human–computer interaction effects [3].

2.1.4. 1969 - Perceptron (artificial neural network)

Mathematical limits identified in simple neural models reduced enthusiasm and funding, triggering an "AI winter" [2].

2.1.5. 1980s - Revival: expert systems and large projects.

Knowledge-based systems and national initiatives (e.g., Japan's Fifth Generation) re-energized research in applied AI and symbolic approaches [2].

2.1.6. 1997- Deep Blue defeats Kasparov (chess).

Landmark showing that specialized search and evaluation systems can outperform top human experts in complex rule-based domains [4].

2.1.7. 2000s - Robotics benchmarks and applied AI

Competitions (RoboCup), better sensors, and increased computational power drive practical robotics and deployed AI services [4].

2.1.8. 2011- Watson wins Jeopardy! (NLP milestone).

Demonstrated large-scale question-answering, advanced NLP pipelines, and integration of heterogeneous knowledge sources [4].

2.1.9. 2012- Deep learning breakthrough (ImageNet / Alex Net).

Convolutional neural networks achieve major gains in vision tasks, signaling the start of the data-driven deep-learning era [5].

2.1.10. 2016 - AlphaGo use reinforcement learning.

AlphaGo Combined deep networks with tree search to master a game long considered beyond programmatic reach [5].

2.1.11. 2018–2020 - Transformer Era and large language models (Generative Pre-trained Transformer, GPT series).

Pre-training and scaling using transformer architecture enabled powerful few-shot and zero-shot language generation and transfer across tasks [5].

2.1.12. 2021 - Multimodal and foundation models

Text–image models (e.g., DALL·E) and large foundation models accelerate cross-domain applications. Thereby AI moves from landmark demos to widespread scientific and commercial use [5].

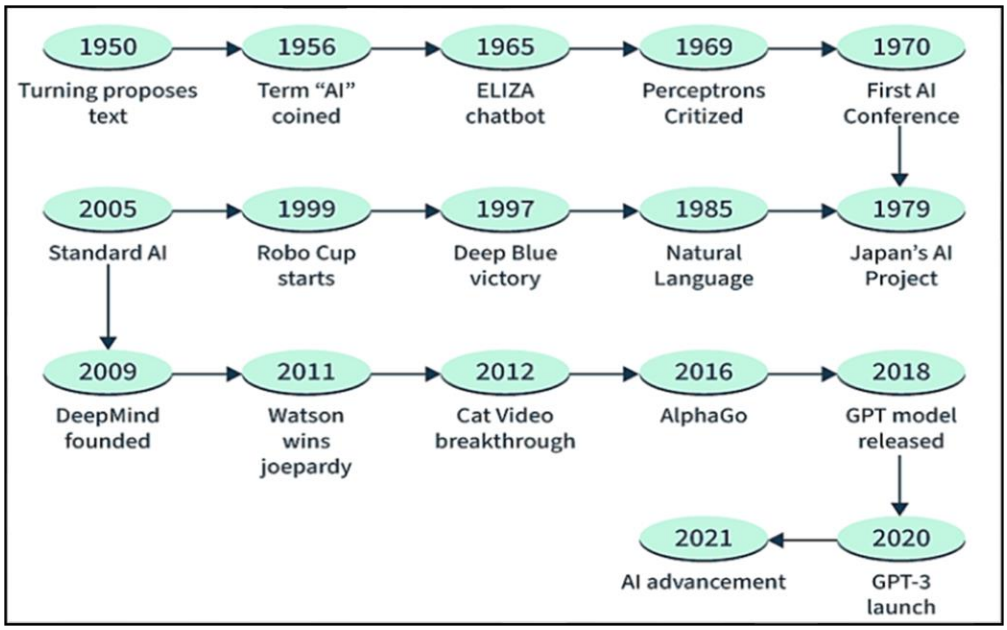

Figure 1 Evolution of AI

3. History of Artificial Intelligence in the Pharmaceutical Field

Artificial Intelligence (AI) has rapidly transformed the pharmaceutical industry, addressing the challenges of high costs, long timelines, and high failure rates in drug development. From its early beginnings with rule-based expert systems in the 1970s to today's deep learning and generative models, AI has become integral across the entire drug discovery and development pipeline. It enables faster target identification, molecule design, clinical trial optimization, and personalized medicine. Tracing the history of AI in pharmaceuticals highlights how technological evolution has shaped modern drug research and continues to redefine future healthcare innovation.

3.1. Early Expert Systems in Chemistry and Medicine

Figure 2 Edward Feigenbaum (Father of Expert Systems)

Artificial intelligence entered pharmaceutical sciences during the mid-20th century with rule-based expert systems. DENDRAL (1960s) assisted organic chemists in predicting molecular structures from mass spectrometry data, marking a milestone in computational chemistry [6]. Early AI research in medicine, such as Edward Feigenbaum's dental

experiments in the 1960s–70s, showed its promise in life sciences [7]. In the 1970s, the MYCIN system applied knowledge-based reasoning to diagnose bacterial infections and recommend antibiotic therapy [8]. Although MYCIN was never clinically deployed due to ethical concerns, both systems established proof-of-concept for AI in medicine, albeit limited by rigid rule sets and computational constraints.

3.2. Bioinformatics and the Genomic Era (1990s–2000s)

The **Human Genome Project (completed in 2003)** generated massive biological datasets, catalyzing AI's use in genomics and molecular biology [9]. Machine learning, a branch of artificial intelligence, enables systems to learn and enhance their performance from experience without requiring explicit programming [10].

- **Identification** (gene–disease associations)
- **Cheminformatics** (QSAR modeling)
- **Molecular docking** (AI-assisted scoring functions).

This period marked a paradigm shift from symbolic reasoning to **statistical learning**, laying foundations for **personalized medicine**, though progress was constrained by fragmented datasets and immature algorithms.

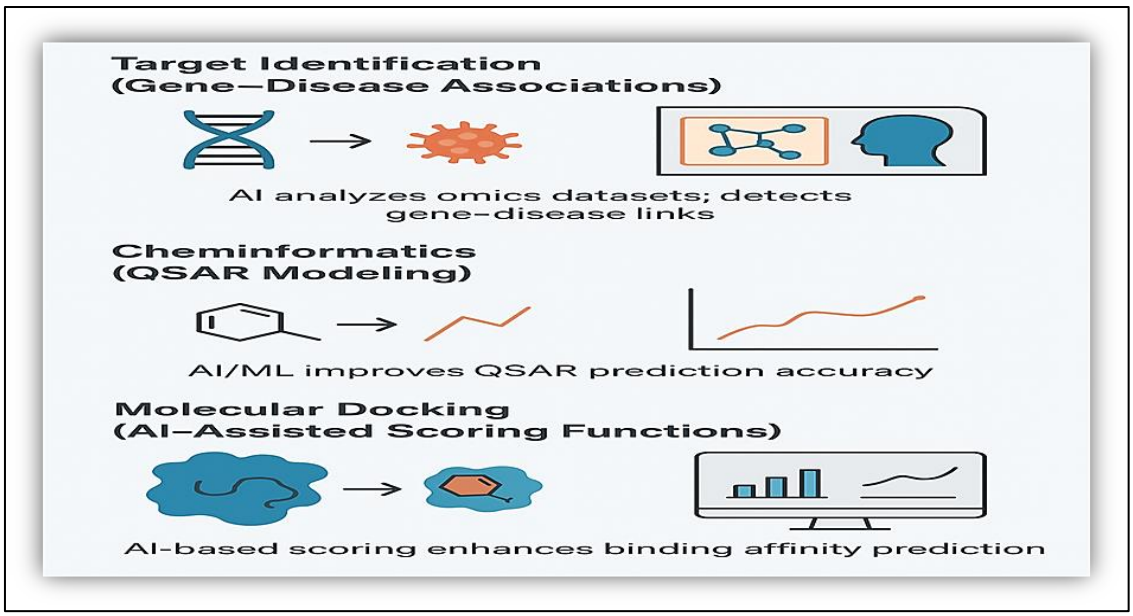

Figure 3 AI In Drug Discovery

3.3. Rise of Machine Learning in Drug Discovery (2010s)

With advances in computing, **deep learning** transformed drug discovery. One landmark development was the application of **convolutional neural networks** to structure-based drug design, enabling more accurate prediction of ligand–protein interactions [11]. Generative models such as **GANs** (generative adversarial network) and reinforcement learning were introduced for de novo molecular design [12]. At the same time, **causal inference frameworks** were applied to model disease mechanisms from high-dimensional clinical and genomic data [13]. These approaches represented a shift from **hypothesis-driven** to **data-driven** drug discovery.

3.4. AI-Driven Antibiotic Discovery: Halicin (2020)

In 2020, researchers used a deep learning model to screen millions of compounds, identifying **Halicin**, the first AI-discovered antibiotic in over 30 years [14]. Halicin exhibited broad-spectrum efficacy, including against multidrug-resistant Acinetobacter baumannii and Mycobacterium tuberculosis [15]. Its novel mechanism—disruption of bacterial proton gradients—distinguished it from traditional antibiotics. Follow-up studies confirmed activity against biofilm-forming pathogens.https://news.mit.edu/2020/artificial-intelligence-identifies-new-antibiotic-0220MITNews.This achievement revitalized antibiotic R&D, historically neglected due to poor commercial incentives.

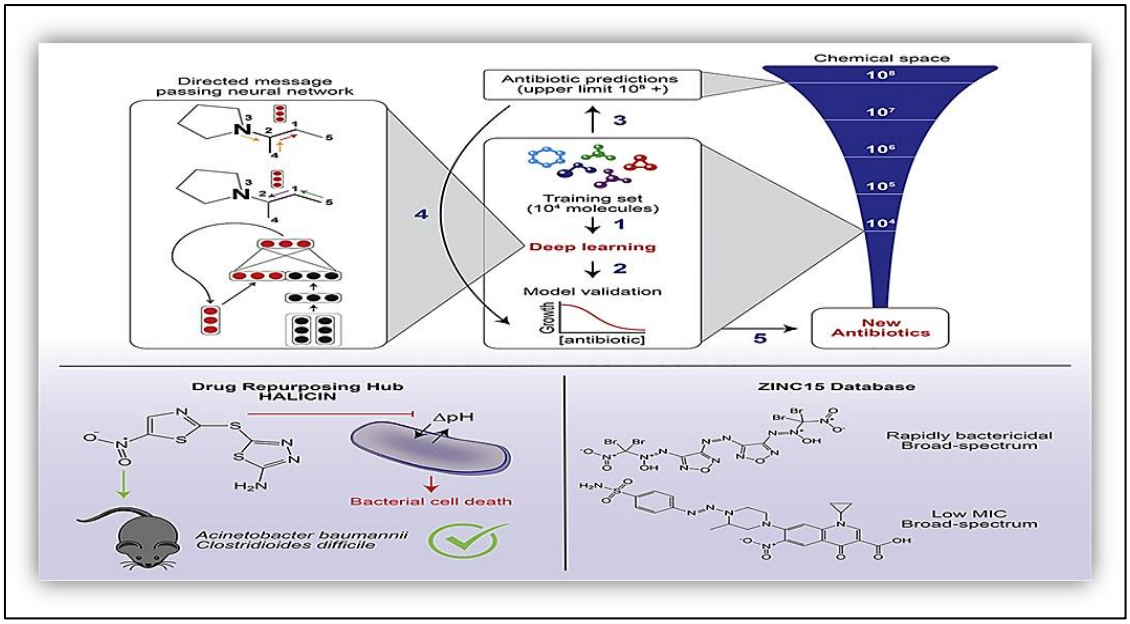

Figure 4 Drug Repurposing and De Novo Antibiotic Discovery Using Deep Learning Models

3.5. AI Platforms for Accelerated Drug Discovery

AI adoption expanded across multiple therapeutic domains, often integrated within design–make–test–learn (DMTL) cycles. Reports suggest that such frameworks can reduce discovery timelines by up to 70% and lower costs substantially https://www.theguardian.com/society/2020/feb/20/antibiotic-that-kills-drug-resistant-bacteria-discovered-through-ai The Guardian . A notable milestone was the development of the first AI-generated small-molecule candidate that advanced from target identification to Phase I clinical evaluation within 12 months [16]. Similarly, an AI-designed compound for fibrotic disease reached Phase II trials in under 30 months, also receiving regulatory recognition https://aws.amazon.com/solutions/case-studies/exscientia-generative-ai/ Amazon Web Services, Inc. . In parallel, high-content imaging combined with ML enabled large-scale phenotypic drug discovery [17]. Collectively, these advances demonstrated that AI could compress R&D cycles from years to months.

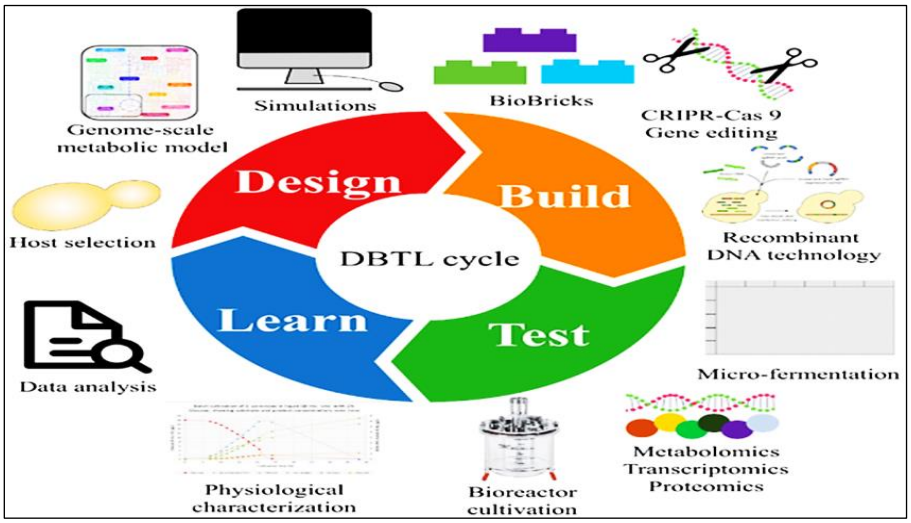

Figure 5 DBTL Framework Integrating Computational and Experimental Methods in Biotechnology

4. Milestones of AI in the Pharmaceutical Science

4.1. Early Computational Approaches

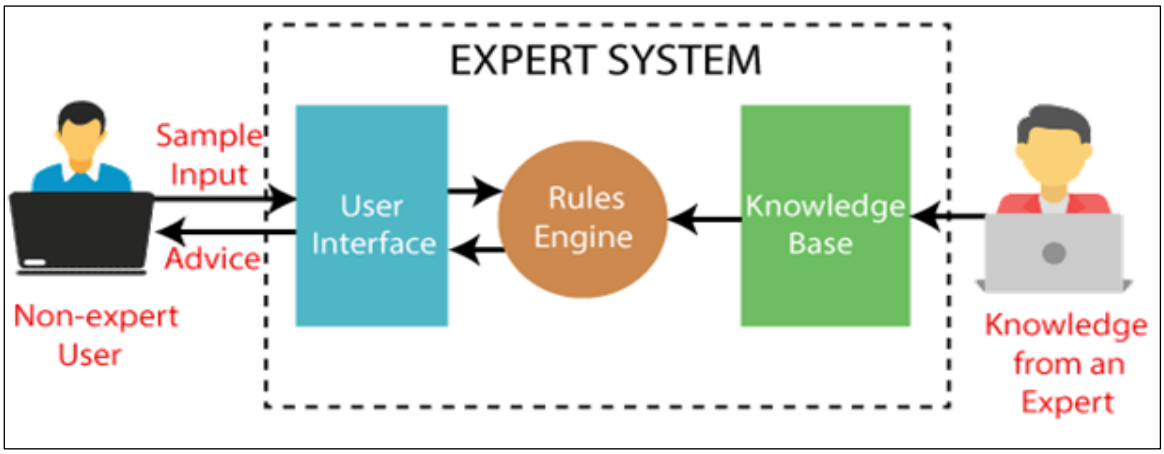

Figure 6 Expert System Work Flow

The first wave of AI in medicine was characterized by rule-based expert systems such as *MYCIN*, which demonstrated the potential of computer-assisted decision-making in clinical practice.

4.2. Drug Discovery and Development

Quantitative structure–activity relationship (QSAR) modeling supported early drug design and optimization [18]. Later advancements automated and accelerated drug discovery pipelines [19]. Virtual screening became pivotal in chemical library screening for candidate molecules [20], with further improvements through deep learning–enhanced docking models [21]. Integration of transcriptomic data with deep learning enabled prediction of pharmacological properties and facilitated drug repurposing [24]. The emergence of *AtomNet* marked a milestone, employing deep convolutional neural networks for bioactivity prediction [25]. AI-driven platforms also enabled rapid identification of novel inhibitors, demonstrating the transformative role of deep learning in structure-based drug design [26].

4.3. Genomics and Personalized Medicine

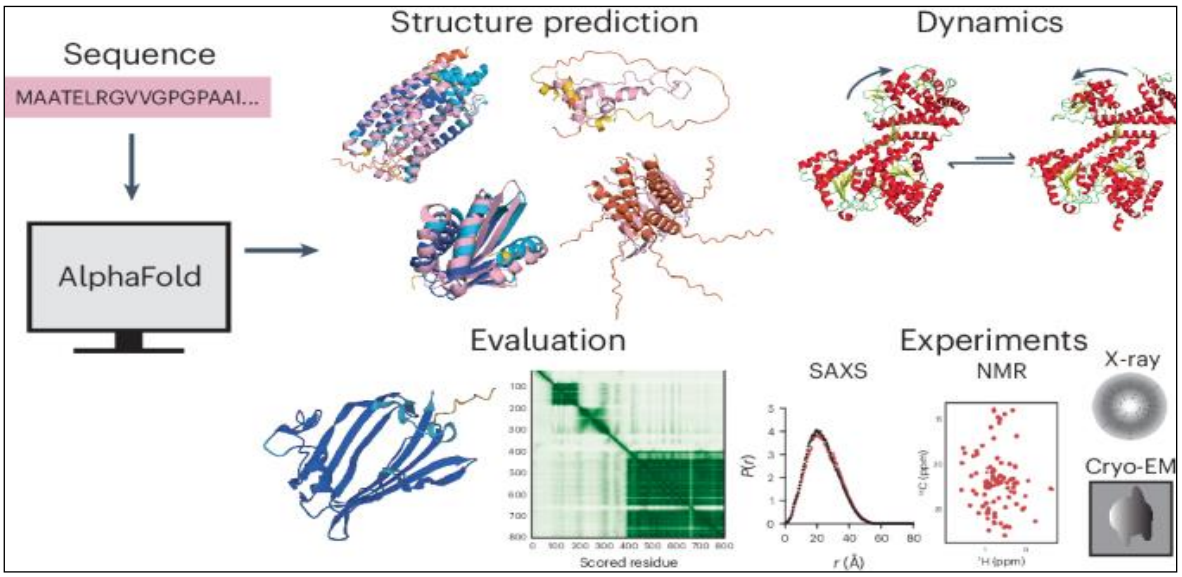

Figure 7 Deep Learning–Based Protein Structure Prediction Using AlphaFold

The sequencing of the human genome provided the foundation for precision medicine [22]. Advances in machine learning extended to genetics and genomics, generating data-driven insights into complex biological mechanisms [23].

Protein structure prediction achieved a breakthrough with *AlphaFold*, which set new benchmarks in accuracy and accelerated personalized therapeutic design [27].

4.4. AI in Manufacturing and Industry 4.0 (Pharma 4.0)

In pharmaceutical manufacturing, AI supports the development of cyber-physical systems aligned with Industry 4.0 principles, improving productivity, traceability, and automation [28]. In industries ranging from space exploration and healthcare to electronics and automobile manufacturing, automation and robotics are indispensable, constantly advancing the limits of research and development [29]. The adoption of IoT will make global supply chains more transparent and efficient [30]. Through IoT, infrastructure components like electricity networks, transport systems, and waste management can be tracked and controlled in real time [31] Data-driven approaches further revolutionize smart manufacturing through predictive maintenance, real-time process control, and quality assurance [32].

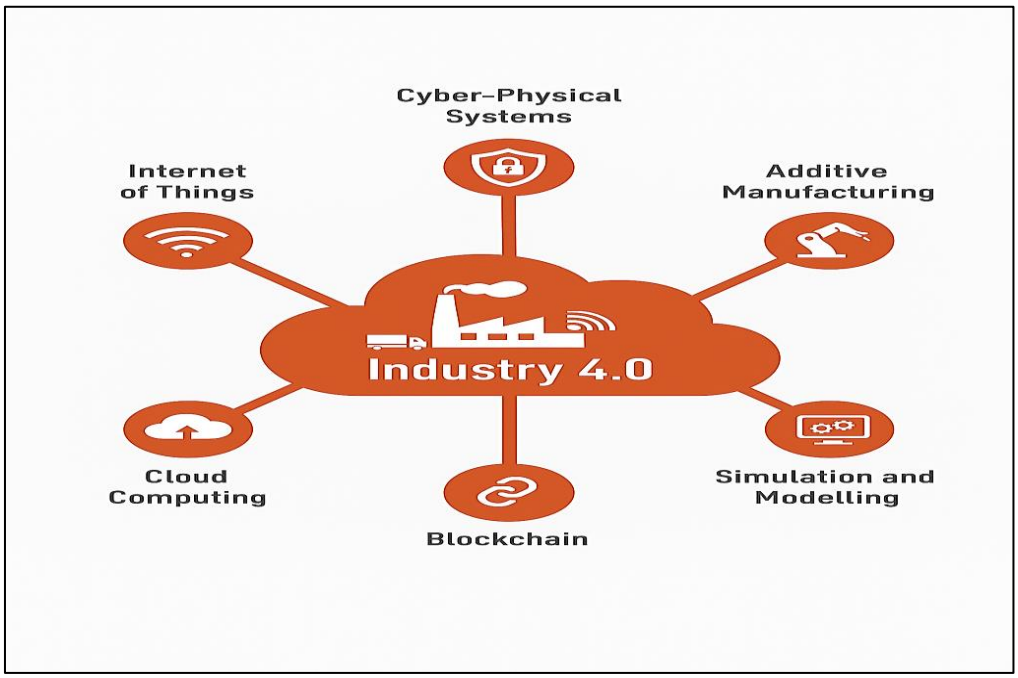

Figure 8 Technological Framework of Industry 4.0

5. The Need for AI Software in the Pharmaceutical Industry

Modern pharmaceutical operations from discovery to post-market surveillance are increasingly data-intensive. High-resolution molecular simulations, multi-omics datasets, electronic health records (EHRs), and patient-reported outcomes collectively form a vast but underutilized information pool [33,34]. Artificial intelligence (AI) techniques including machine learning (ML), natural language processing (NLP), and predictive modeling transform this unstructured data into actionable knowledge [35,36]. In an era where speed-to-market, cost efficiency, and patient safety are paramount, AI adoption is no longer optional but essential [37].

5.1. Sluggish and Costly R&D

The average cost of bringing a new drug to market often exceeds USD 2.6 billion, with high attrition rates across the pipeline [38]. AI-driven predictive models can filter out non-viable compounds early, saving both time and resources. Advanced deep generative models can even propose novel chemical structures with optimized pharmacokinetic properties before synthesis, accelerating the discovery process [35].

5.2. Manufacturing Variability and Compliance Risk

Manual monitoring in Good Manufacturing Practice (GMP) environments frequently delays error detection. AI-enabled real-time analytics identify micro-variations in process parameters, enabling corrective interventions before deviations escalate [39]. Furthermore, predictive maintenance reduces downtime, and AI-driven batch release systems streamline quality control by integrating results instantly [36].

5.3. One-Size-Fits-All Therapies

Conventional therapies often ignore patient-specific biological variability [40]. AI-powered multi-omics platforms integrate genomics, proteomics, and metabolomics to guide the design of personalized therapies, thereby improving success rates [41]. In particular AI-assisted biomarker identification has proven especially valuable in immuno-oncology drug development [33].

5.4. Delayed Safety Signals

Adverse drug events (ADEs) typically become visible only after large-scale clinical use [42]. AI-enabled pharmacovigilance systems continuously scan scientific literature, patient forums, and even social media to detect early warning signals, strengthening drug safety surveillance [38].

5.5. Strategic Impact

AI adoption fundamentally transforms pharmaceutical workflows from linear, reactive processes into adaptive, proactive systems (https://www.fda.gov/medical-devices/software-medical-device-samd/artificial-intelligence-and-machine-learning-software-medical-device U.S. Food and Drug Administration). By enhancing predictive accuracy, operational agility, and regulatory preparedness, AI has shifted from being a competitive advantage to becoming a survival necessity for modern pharmaceutical enterprises [37].

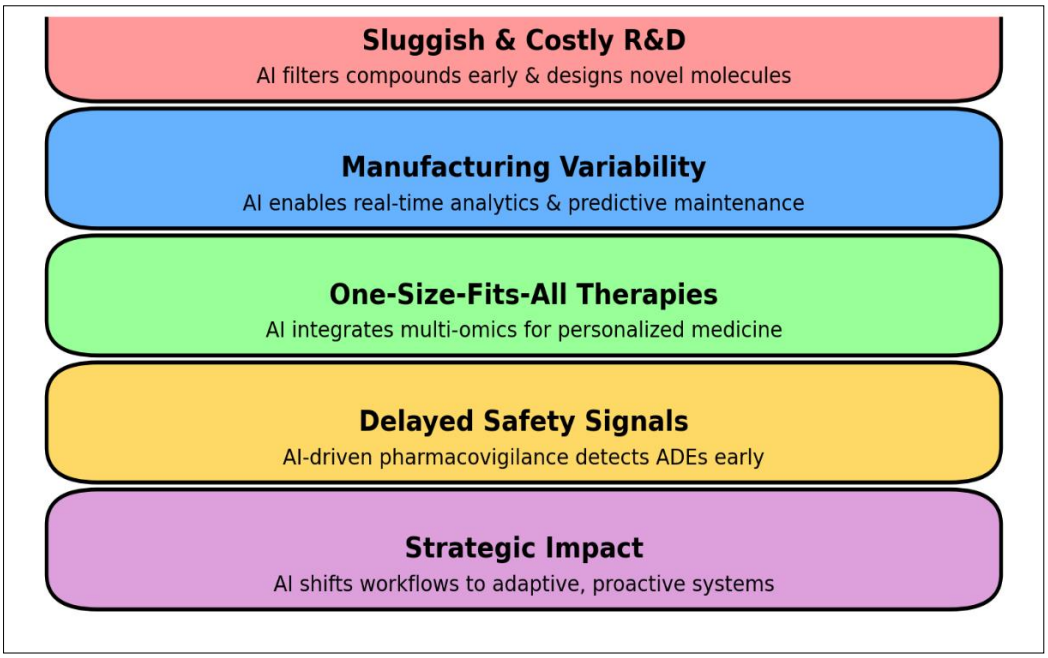

Figure 9 Role of Artificial Intelligence in Addressing Key Challenges of the Pharmaceutical Industry

6. AI Software in Pharmaceutical Industry

Artificial Intelligence (AI) software is transforming the pharmaceutical industry by speeding up drug discovery, boosting clinical trials, and enhancing patient safety. By analyzing massive biomedical and clinical datasets, AI helps reduce costs, save time, and support personalized medicine. It is now a key driver of innovation in modern healthcare.

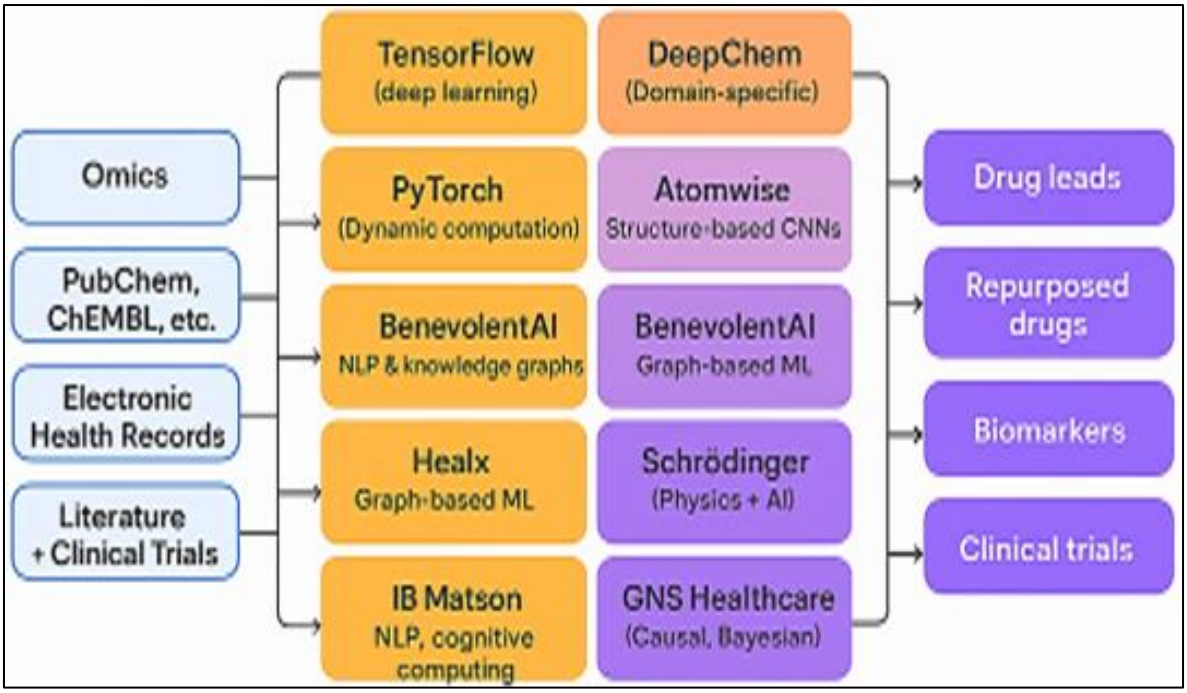

Figure 10 AI Software Applications in the Pharmaceutical Industry

Table 1 AI software for Small-Molecule Drug Discovery and Drug Design

Ai Software	Principle Function	Therapeutic Focus	Drug Development Phase	Key Outcomes
Atomwise	Docking studies	Oncology, Infectious diseases (Ebola)	Drug discovery and Preclinical phase	Identified small-molecule inhibitors against Ebola virus polymerase and oncology targets [43]
Exscientia	AI- driven drug design	CNS disorders (Bipolar and OCD disorders)	Drug Discovery to Clinical phase	AI-designed small-molecule drug (DSP-1181) for obsessive-compulsive disorder (OCD), which entered Phase I clinical trials in 2020 [44]
Insilico Medicine	Generative chemistry and Target ID	Fibrosis	Drug Discovery to Clinical phase	AI identified a novel TNIK inhibitor for idiopathic pulmonary fibrosis (IPF) [45]
Schrödinger	Computational chemistry and Molecular dynamics	Oncology, CNS disorders	Drug Discovery and Preclinical Phase	Accelerated drug design via Quantum Mechanics and Molecular Dynamics. https://www.schrodinger.com

Table 2 AI software for Protein Design and Advanced Therapeutics

AI Software	Principle function	Therapeutic Focus	Drug Development phase	Key outcomes
Isomorphic Labs (Alphabet)	Protein Structure Prediction, Drug Target Identification	Neurodegenerative disorders (Alzheimer, Parkinson), Oncology	Drug Discovery and Preclinical phase	Applied AlphaFold for structure-guided design [46]
AION Labs (Alliance for Innovation Laboratories)	AI-enabled Antibody Engineering and Targeted Protein Degradation Inducers	Oncology	Drug Discovery and Preclinical phase	Created DenovAI (antibody platform) and TenAces (molecular glue platform) https://aionlabs.com
Linguamatics (IQVIA)	Natural Language Processing and Biomedical Text Mining Tool	Multiple areas (cardiology, Oncology, neurology)	Drug Discovery and Preclinical phase	It extracts knowledge from scientific literature, clinical trial registries, patents, and electronic health records. https://www.linguamatics.com

6.1. Future outlook

AI is set to move from a supportive role to a core driver of pharmaceutical innovation. Generative models will design novel compounds, while integration with robotics, digital twins, and automation will create self-optimizing laboratories. In drug discovery, AI will combine multi-omics data to improve target identification, patient stratification, and clinical trial success. On the clinical side, AI will accelerate the shift toward personalized medicine, using genomic and real-world data to tailor treatments. In manufacturing, convergence with Pharma 4.0 and IoT will enable real-time monitoring, predictive maintenance, and cost-efficient production of biologics.

Future progress, however, depends on addressing bias, data interoperability, and regulatory trust. With responsible adoption, AI will evolve into an intelligence layer that underpins every stage of drug development, reducing costs, shortening timelines, and expanding therapeutic possibilities.

7. Conclusion

The history of Artificial Intelligence in the pharmaceutical field demonstrates a clear evolution from symbolic reasoning systems to data-driven deep learning and generative models. Each technological leap has reduced barriers in drug discovery, accelerated timelines, and improved predictive accuracy. Today, AI not only supports target identification and drug design but also optimizes clinical trials, ensures manufacturing quality, and enhances patient safety through pharmacovigilance. As pharmaceutical enterprises move into the era of Pharma 4.0, AI adoption is no longer optional but essential. Its integration promises more cost-effective, precise, and patient-centered therapies. Looking ahead, the fusion of AI with multi-omics, robotics, and real-world data will continue to redefine the landscape of drug research and healthcare delivery.

Compliance with ethical standards

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Disclosure of conflict of interest

The authors have no conflicts of interest regarding this investigation.

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