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*Review Article*

# Artificial Intelligence in the Pharmaceutical Industry: Innovating Drug Discovery, Clinical Trials, and Supply Chains

**Lavanya Sawarkar, Nisha Fungal, Vedika Shinde, Prashant Chaturvedi, Yogesh Wankhede***

*MET's Institute of D. Pharmacy, Bhujbal Knowledge City, Adgaon, Nashik 422003, Maharashtra, India*

Few corners of the pharmaceutical sciences have been left untouched by artificial intelligence, but nowhere is the effect more visible than in the pipeline that runs from a candidate molecule to an approved therapy. Machine learning (ML), deep learning (DL), and related computational techniques are now routinely applied to drug discovery, pre-clinical research, pharmaceutical manufacturing, supply chain management, and clinical trial optimization, and this review pulls together what the current literature says about where those applications actually stand (1,2,3). The picture that emerges is genuinely encouraging in places: AI-enabled platforms have shortened discovery timelines, sharpened predictions of compound efficacy and toxicity, and streamlined patient recruitment for trials. The commercial numbers tell a similar story, if a somewhat inconsistent one — the global market for AI in drug discovery has been valued at anywhere between roughly US$1.5 and US$3.5 billion as of 2023, depending on the analysis, with projected annual growth of 12-30% through 2030 (1). Sanofi, Pfizer, Novartis, and AstraZeneca are among the major companies that have each built dedicated AI partnerships or in-house platforms to accelerate research and development (1,3). Yet the literature is equally clear that these gains have not yet translated cleanly into safe, reliable therapeutics at scale. Regulatory frameworks remain fragmented across jurisdictions, many of the underlying models are still opaque "black boxes," questions of accountability when an AI-informed decision causes harm remain largely unresolved, and data quality and standardization problems persist throughout the pipeline (1,2). Closing that gap, this review argues, will take harmonized regulation, rigorous validation standards, and sustained collaboration between industry, academia, and regulators — rather than further gains in model performance alone.

**Keywords**: Artificial intelligence, Pharmaceutical Industry, Innovating Drug Discovery, Clinical Trials, Supply Chains.

## INTRODUCTION

Artificial intelligence is, at its core, the branch of computer science concerned with getting machines to do things that would ordinarily require human intelligence — learning, reasoning, perceiving, solving problems. Alan Turing gave the field its founding question in 1950, in "Computing Machinery and Intelligence," and John McCarthy later gave it a working definition in 2004: the science and engineering of building intelligent machines. In the seven decades between those two milestones, AI moved from brittle, rule-based expert systems to the deep learning architectures now capable of chewing through vast, messy, heterogeneous datasets (2) Nowhere has that evolution been more heavily capitalized than in pharmaceutical research. The global AI-in-drug-discovery market was valued at roughly US$1.5 billion in 2023, on track, by one estimate, for a 29.7% compound annual growth rate and a US$11.8 billion valuation by 2030; a separate analysis puts the 2023 figure closer to US$3.54 billion, growing more modestly to US$7.94 billion by 2030 at a 12.2% CAGR. The two estimates disagree sharply on the specifics, but they agree on the headline: this is now one of the most heavily funded

corners of pharmaceutical innovation (1). What follows focuses narrowly on that industrial and developmental side of the story — how AI is used to discover, test, manufacture, and eventually bring new therapies to market, and how deeply major pharmaceutical companies have woven these tools into their R&D strategy. A companion review takes up the other half of the question: what happens once a medicine leaves the factory and reaches a pharmacist and a patient. This paper stays upstream of that point. Its aim is to pull together what the literature says about AI's role in drug discovery, clinical trials, and industry adoption, and to look hard at the technical, regulatory, and ethical obstacles standing between today's promising results and something genuinely reliable and generalizable.

## SCOPE AND OBJECTIVES

This review is deliberately bounded to the upstream, pre-dispensing segment of the medicine lifecycle. It does not address clinical decision support, medication dispensing, adherence, or direct patient care, each of which is addressed in a separate companion review. Within this bounded scope, the paper pursues three objectives:

- To evaluate the extent to which AI improves the efficiency of therapeutic development, including reductions in the time and cost required to identify, test, and manufacture new medicines.
- To analyze the structural changes AI is introducing to industrial drug pipelines, including discovery, pre-clinical testing, manufacturing, supply chain management, and clinical trial design.
- To critically appraise the regulatory, technical, and ethical barriers — including data standardization, algorithmic opacity in trial decision-making, and fragmented international approval frameworks — that must be resolved before these industrial gains can be considered safe and generalizable.

## CLASSIFICATION OF ARTIFICIAL INTELLIGENCE

AI systems are commonly classified according to the caliber, or level, of intelligence they exhibit. Artificial narrow intelligence (ANI) describes systems designed and trained to perform a single, narrow task, such as facial recognition or predicting molecular binding affinity; virtually all AI currently deployed in pharmaceutical research falls into this category. Artificial general intelligence (AGI) would replicate the full range of human intellectual abilities, while artificial super intelligence (ASI) describes a hypothetical form of intelligence exceeding human cognitive capacity across every domain; neither has yet been realized (3). A complementary scheme, proposed by the AI scientist Arend Hintze, classifies systems by their existing or potential capabilities. "Reactive machine" systems identify patterns and make predictions but retain no memory of past experience, as exemplified by IBM's Deep Blue chess programmed. "Limited memory" systems draw on past observations to inform present decisions; a capability increasingly used in predictive modelling for drug candidate screening. The more advanced "theory of mind" and "self-awareness" categories remain theoretical and have no current application in pharmaceutical development (3). These foundational distinctions are useful in the discussion that follows, since the majority of tools described in this review — from molecule-screening platforms to clinical trial recruitment algorithms — are narrow, task-specific systems rather than general-purpose reasoning agents.

### AI In Drug Discovery And Development

The clearest way to see AI's impact on the discovery pipeline is to look at speed and precision together. Machine learning models now predict compound efficacy and safety profiles well enough to streamline early-stage development and to make repurposing existing drugs for new indications a genuinely practical strategy cutting into the time and cost that have historically made bringing a new therapy to market such a slow, expensive process (1).

## DISCOVERY, PRE-CLINICAL RESEARCH, AND MANUFACTURING

During the discovery phase, AI facilitates the identification of drug candidates by analyzing extensive datasets of chemical compounds and predicting their efficacy, while also supporting the repurposing of existing drugs for new indications. In pre-clinical research, AI-based simulations of biological processes reduce reliance on animal

models and accelerate the analysis of safety and toxicity data. During manufacturing, AI continuously monitors and optimizes production processes to ensure consistent drug quality, while predictive maintenance algorithms anticipate equipment failures before they occur (1). Reviews of the field describe this as a genuine paradigm shift in how candidate molecules are identified and prioritized, even as they caution that the gap between promising in-silico predictions and validated in-vivo results remains a persistent source of attrition (12), a concern echoed in assessments of AI's role specifically in the earliest, most exploratory stages of the discovery pipeline (13). Several companies illustrate the practical application of these techniques. Atom wise has applied deep learning neural networks, including its Atom Net platform, to predict the binding properties of small molecules to protein targets using three-dimensional structural representations, compressing hit discovery, lead optimization, and toxicity prediction into a matter of weeks rather than years. Insilco Medicine has applied generative adversarial networks (GANs) and reinforcement learning to generate novel molecular structures and to hypothesized the biological origins of disease (3). A 2022 assessment in Nature Reviews Drug Discovery reached a more measured verdict, noting that while AI-native companies were already broadening the diversity of molecules under investigation and improving early-stage productivity, no AI-discovered drug had at that point received regulatory approval, and the technology's real test would come only once the first cohorts reached late-stage trials (7). Target identification has followed a similar trajectory: AI methods that integrate diverse biological data modalities have improved the prediction of drug target properties and illuminated disease mechanisms, though model interpretability, data bias, and the downstream validation of predicted targets remain unresolved obstacles (8). Broader surveys of the field reach a consistent conclusion: machine learning and deep learning have been applied across essentially every stage of the discovery pipeline, from peptide synthesis and virtual screening to toxicity prediction and drug repositioning, though the underlying models still depend heavily on the volume and quality of the biological, chemical, and clinical data available to train them (10,14,15), a point echoed in a widely cited 2019 review of machine-learning applications across the discovery and development pipeline (11).

**Supply Chain Management**

Supply chains are one of the less glamorous places AI has made a real dent. Better demand forecasting, tighter inventory levels, and faster disruption response all come out of the same predictive-analytics toolkit, and manufacturers who use it are simply better at anticipating swings in demand which means fewer stockouts, less surplus stock sitting unused, and better allocation of resources overall (1).

- **Inventory optimization:** machine learning algorithms analyses usage data to maintain optimal stock levels, minimize holding costs, and ensure regulatory compliance (1).
- **Real-time disruption management:** AI enhances visibility across the supply chain, enabling organizations to respond swiftly to disruptions, while automation and robotics reduce human error (1).

**Post-Market Surveillance**

At the industry level, AI supports post-marketing pharmacovigilance by monitoring adverse drug reaction reports and tracking emerging safety signals across healthcare systems and social media platforms, contributing to a more proactive surveillance strategy at scale. The clinical detection of individual adverse drug reactions at the point of care is addressed in the companion review of clinical pharmacy practice (1).

**AI in Clinical Trials**

Clinical trials are notoriously slow, and a lot of that slowness comes down to three things: finding the right patients, watching them closely enough once enrolled, and identifying the biomarkers that actually matter. AI has made inroads on all three. Predictive analytics draw on historical data to sharpen trial design including dosage levels and cohort selection which tends to mean faster, more accurate outcomes at lower cost (1). On recruitment specifically, AI tools that scan electronic health records can identify eligible candidates far faster than a human reviewer working through charts by hand, and predictive models that stratify patients by genetic and clinical profile tend to

improve who actually gets enrolled. In trials for age-related macular degeneration, for instance, AI-assisted screening outperformed manual selection on precision. Natural language processing does something similar with unstructured records, matching patients against eligibility criteria with less manual effort and, generally, better accuracy (1). The gains aren't confined to recruitment, either. Continuous data analysis lets trial teams adjust protocols in real time and try designs that would have been impractical under older, static approaches, while AI-driven monitoring helps catch problems early enough to intervene. Simulation and predictive modelling cut down on how much experimental testing is needed in the first place, which shortens timelines, and AI-assisted biomarker identification threads through recruitment, monitoring, and outcome prediction all at once (1). None of this comes free of complications, though. Folding AI into trial processes raises real technical, regulatory, ethical, and operational questions data quality and standardization chief among them, along with how well these systems interoperate with the trial infrastructure already in place. And the "black-box" nature of many of these models doesn't help: when it's hard to say why a model reached a given conclusion, that's a genuine obstacle to stakeholder trust, one that only rigorous validation protocols can really address (1).

**Industry Adoption: Major Pharmaceutical Companies**

Major pharmaceutical companies are increasingly collaborating with, or acquiring, AI technology vendors to embed AI within research, development, and manufacturing processes. Reports indicate that nearly 62% of healthcare organizations are considering AI investment in the near term, and 72% believe AI will be crucial to how they conduct business in the future; the McKinsey Global Institute has estimated that AI and machine learning could generate close to US$100 billion annually across the United States healthcare system (3). A 2026 survey of the vendor landscape counted well over 150 companies actively supplying AI tools across discovery, clinical development, and manufacturing, suggesting the market has moved well beyond a handful of headline partnerships into a genuinely crowded ecosystem (9). The roll call of partnerships is long, and it keeps growing. Sanofi built its own "Plai" platform to support discovery, trials, and manufacturing in-house. Pfizer has leaned on IBM's supercomputing and AI capabilities since 2020, work that fed into the oral COVID-19 treatment Paxlovid, approved in 2022. Novartis has partnered with Microsoft and NVIDIA with an eye toward scaling AI use over the next decade, and Janssen is exploring applications across discovery, trials, diagnosis, and manufacturing all at once. AstraZeneca teamed up with Onco shot in 2021 to match patients to trials using AI, and separately with Benevolent AI on novel drug targets; Bristol Myers Squibb and Bayer have each gone to Ex Scientia for small-molecule discovery work spanning oncology and immunology (1). In 2018, the Massachusetts Institute of Technology partnered with Novartis and Pfizer to transform drug design and manufacturing through its Machine Learning for Pharmaceutical Discovery and Synthesis Consortium, and additional major companies, including Roche, Merck, GlaxoSmithKline, AbbVie, and Johnson & Johnson, have separately collaborated with or acquired AI technology providers. These industry-wide collaborations illustrate the transformative role AI is playing in developing new therapies and fostering a more efficient, data-driven approach to pharmaceutical development (1,3). This enthusiasm has nonetheless been tempered by market correction. Valuations for many AI-focused drug discovery firms have declined substantially since the wave of 2021-2022 IPOs, and industry commentary entering 2026 describes a period of consolidation in which better-capitalized platforms acquire distressed assets while weaker entrants exit the market; whether this recalibration reflects a maturing sector or persistent doubts about AI's ability to improve clinical success rates remains an open, closely watched question (5). A separate 2026 industry analysis frames the same period more narrowly around intellectual property, arguing that the firms weathering the correction best are those that have translated AI-generated leads into defensible, patentable assets rather than those that simply generated the largest volume of candidate molecules — a reminder that computational productivity and commercial value are not the same thing (6).

## CHALLENGES AND RISKS IN AI-ENABLED DEVELOPMENT

### Regulatory Uncertainty

Regulation has had a hard time keeping up. Traditional clinical trial approval processes were built for a world of fixed, static interventions, not for machine learning algorithms that keep updating as new data comes in, and that mismatch complicates how safety and efficacy get assessed for AI-driven decision-making systems. Get the validation wrong and the risks are real misdiagnosis, incorrect patient stratification, unreliable clinical advice. Because trials increasingly run across borders, the case for harmonized international standards is strong; the European Union has moved furthest with its AI Act, but most other jurisdictions still lack an equivalent framework, and that patchwork drives up costs, delays trials, and limits how far AI innovations can scale (1). A first real step toward closing that gap came in January 2026, when the FDA and the European Medicines Agency jointly published ten guiding principles for good AI practice spanning the entire drug development lifecycle — from non-clinical research through trials to manufacturing and post-marketing surveillance. It's the first transatlantic alignment specifically aimed at AI in pharmaceutical development (4).

### Explainability And Accountability

A separate but related problem is that many of the models used in discovery and trial design are still opaque — genuine "black boxes" whose reasoning is hard to reconstruct after the fact. That's not just an inconvenience; it erodes trust among developers, clinicians, and regulators alike, and it's part of why rigorous validation protocols matter so much before deployment. It also raises an accountability question nobody has fully answered: when an AI-informed decision leads to a costly or harmful outcome, who is responsible the organization that developed it, the vendor who built the underlying software, or the regulator who signed off on it (1,2) Several documented cases illustrate the consequences of these risks. IBM's Watson for Oncology faced widespread criticism after delivering inaccurate or unsafe treatment recommendations, a failure attributed to incomplete or non- representative training data, while at least one high-profile AI-driven clinical trial failed outright because of inaccurate predictions of patient outcomes, resulting in wasted resources and delays to drug development. These cases underscore the importance of transparency mechanisms that allow AI-supported decisions to be audited, alongside representative training data and meaningful stakeholder engagement throughout the design and implementation process (1).

### Data Quality and Technical Barriers

AI systems require high-quality, standardized, and diverse datasets to function optimally. A lack of standardized data formats, combined with the need for extensive data curation, can hinder AI's ability to deliver accurate insights, while integrating AI systems with existing research and trial infrastructure is complicated by variation in system architecture. Overfitting represents a further technical risk, occurring when a model learns spurious relationships between variables and outcomes as a result of having too many parameters relative to the available data (1,2).

## FUTURE DIRECTIONS

- Optimizing supply chain management: leveraging predictive analytics on historical sales, seasonal trends, and local health data to enable more precise forecasting of medication demand and evaluation of supplier reliability (1).
- Harmonizing regulatory frameworks: extending AI-specific safety and validation standards, comparable to the European Union's AI Act, across additional jurisdictions to reduce trial delays and enable scalable, cross-border AI adoption (1).
- Strengthening explainability standards: developing auditable, interpretable models for trial design and discovery, to build the stakeholder trust needed for wider regulatory acceptance (1).
- Deepening industry-academic collaboration: expanding consortium-based models, following examples such as the MIT-Novartis-Pfizer partnership, to accelerate validated, transparent AI tools for pharmaceutical development (1,3).

## LIMITATIONS OF THIS REVIEW

This review draws primarily on a small number of secondary literature reviews rather than a systematic, protocol-driven search of primary studies, so it should be read as a synthesis of existing overviews rather than an exhaustive or independently verified account of the primary evidence base. No formal quality appraisal (such as a risk-of-bias assessment) was applied to the underlying sources, and figures on market size, growth rates, and industry investment vary considerably between the reports cited, reflecting genuine disagreement in the field rather than an error in this review. The pace of change in this area is also worth flagging directly: several of the developments discussed, including the FDA-EMA guiding principles and the 2026 market correction in AI-native drug discovery firms, are recent enough that their long-term significance is not yet settled, and readers should treat forward-looking claims in Section 7 as informed extrapolation rather than established fact.

## CONCLUSION

Pull back far enough, and the story this review has told is fairly simple: AI is leaving its mark on nearly every stage of pharmaceutical development, from the first candidate molecule through pre-clinical testing, manufacturing, supply chain management, and clinical trial design. The tools reviewed here have measurably cut the time and cost of bringing New therapies to market, and that track record has been enough to draw major financial investment and strategic partnerships across the industry (1,3). What's far less settled is whether those gains can be turned into consistently safe, reliable medicines rather than impressive pilot results. Regulatory oversight is still fragmented, many of the models remain hard to interpret, accountability when something goes wrong is still an open question, and data quality issues keep surfacing across the pipeline. None of that resolves itself; it takes coordinated work from developers, regulators, and academic partners, and it takes harmonized international standards and validation frameworks that don't yet fully exist (1,2). Readers interested in what happens once these AI-informed therapies reach the pharmacist and the patient clinical decision support, dispensing, adherence, and direct patient care are directed to the companion review, Artificial Intelligence in Clinical and Community Pharmacy Practice: Transforming Medication Safety and Patient Care.

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