

Artificial Intelligence and Digital Twins used in Pharmaceutical. Research and Practice

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Abstract

Artificial intelligence (AI) and digital twin (DT) technologies are converging to reshape pharmaceutical research and practice — from in-silico target identification and preclinical safety testing, through virtualized clinical trials and personalized therapeutics, to smarter manufacturing and supply-chain resilience. This review summarizes current capabilities, representative applications, technical approaches, regulatory status, challenges, and near-term directions, with concrete examples and key references for further reading.

1. Introduction

Artificial Intelligence (AI) here denotes machine learning (ML), deep learning (DL), and generative models applied to pattern discovery, prediction, simulation, and decision support across the drug lifecycle.¹

Digital Twin (DT) denotes a computational, dynamically updated virtual replica of a real physical entity (e.g., a patient, a process line, or a drug product batch) that can be used for simulation, what-if analysis, optimization and control. DTs for pharma range from process digital twins (manufacturing lines, PAT—process analytical technology) to patient/virtual-patient twins used in trial simulation and precision dosing.²

In that connection, digital twins are a big deal—they're one of the best tools for simulating and improving processes. They create a virtual copy of a real-world system, like a machine or production line, and show ex³

how it behaves in real time. This helps in industries like manufacturing and pharmaceuticals, where things can go wrong. Companies can check many production lines, test different situations, and spot problems before they cause big issues. This leads to more reliable operations. Building on this, Smart Pharma TwinNet uses powerful AI to make digital twins even better. It looks at data from sensors to understand how machines are doing and what's happening in production.⁴

It can spot unusual patterns and help teams take action early to keep quality under control.⁵

Advantages of AI and Digital Twins in Pharmacy Research and Practice

1. Drug Discovery and Development

- AI analyzes large biological and chemical data to identify new drug molecules faster.⁶
- Digital twins simulate drug–target interactions before laboratory testing.
- Reduces time, cost, and failure rate of drug development.⁷

2. Personalized Medicine

- AI helps design patient-specific drug therapy based on genetics and clinical data.
- Digital twins of patients predict individual drug response and side effects.
- Improves treatment safety and effectiveness.⁸

3. Clinical Trials Optimization

- AI selects suitable patients and predicts trial outcomes.
- Digital twins simulate clinical trials, reducing the need for extensive human trials.
- Increases success rate and ethical safety.⁹

4. Improved Drug Formulation

- AI predicts stability, bioavailability, and dissolution behavior of formulations.
- Digital twins model manufacturing processes for tablets, capsules, and gels.
- Enhances product quality and consistency.¹⁰

5. Predictive Safety and Toxicity

- AI detects potential toxicity and adverse drug reactions early.¹¹
- Digital twins simulate long-term drug effects on organs.
- Improves patient safety.

6. Quality Control and Manufacturing

- AI monitors production in real time and detects defects.
- Digital twins optimize manufacturing parameters.
- Ensures GMP compliance and reduces batch failures^{12,13}

7. Faster Research and Innovation

- Automates data analysis and literature review.
- Enables virtual experiments, saving time and resources.
- Encourages innovation in pharmaceutical research.

8. Cost and Resource Reduction

- Minimizes laboratory experiments and clinical failures.
- Reduces wastage of raw materials.
- Lowers overall R&D costs.

9. Enhanced Pharmacovigilance

- AI continuously monitors adverse drug reaction databases.
- Digital twins help understand drug behavior post-marketing.
- Improves drug safety monitoring.

10. Better Decision-Making in Pharmacy Practice

- AI supports clinical pharmacists in dose adjustment and drug selection.
- Digital twins assist in therapy optimization.
- Leads to improved patient outcomes.¹⁴

Disadvantages of Artificial Intelligence (AI) in Pharmacy Research & Practice

1. High Initial Cost

AI systems require expensive software, hardware, and skilled professionals.

2. Data Privacy and Security Issues

Patient data used by AI may be misused, hacked, or leaked if not properly protected.

3. Dependence on Data Quality

AI results are only as good as the data provided. Poor or biased data leads to wrong outcomes.

4. Lack of Transparency (Black Box Problem)

Many AI models do not clearly explain how decisions are made, reducing trust.

5. Ethical and Legal Concerns

Issues related to accountability, consent, and patient safety may arise.¹⁵

Disadvantages of Digital Twins in Pharmacy Research & Practice

1. Complex Development

Creating accurate digital twins of biological systems or patients is difficult.¹⁶

2. High Implementation Cost

Requires advanced sensors, data integration, and computing infrastructure.

3. Data Integration Challenges

Combining real-time clinical, biological, and manufacturing data is challenging.

4. Limited Accuracy in Biological Systems

Human biology is complex; digital twins may not fully represent real patient responses.¹⁷

5. Technical Expertise Required

Highly skilled professionals are needed to develop and maintain digital twins.

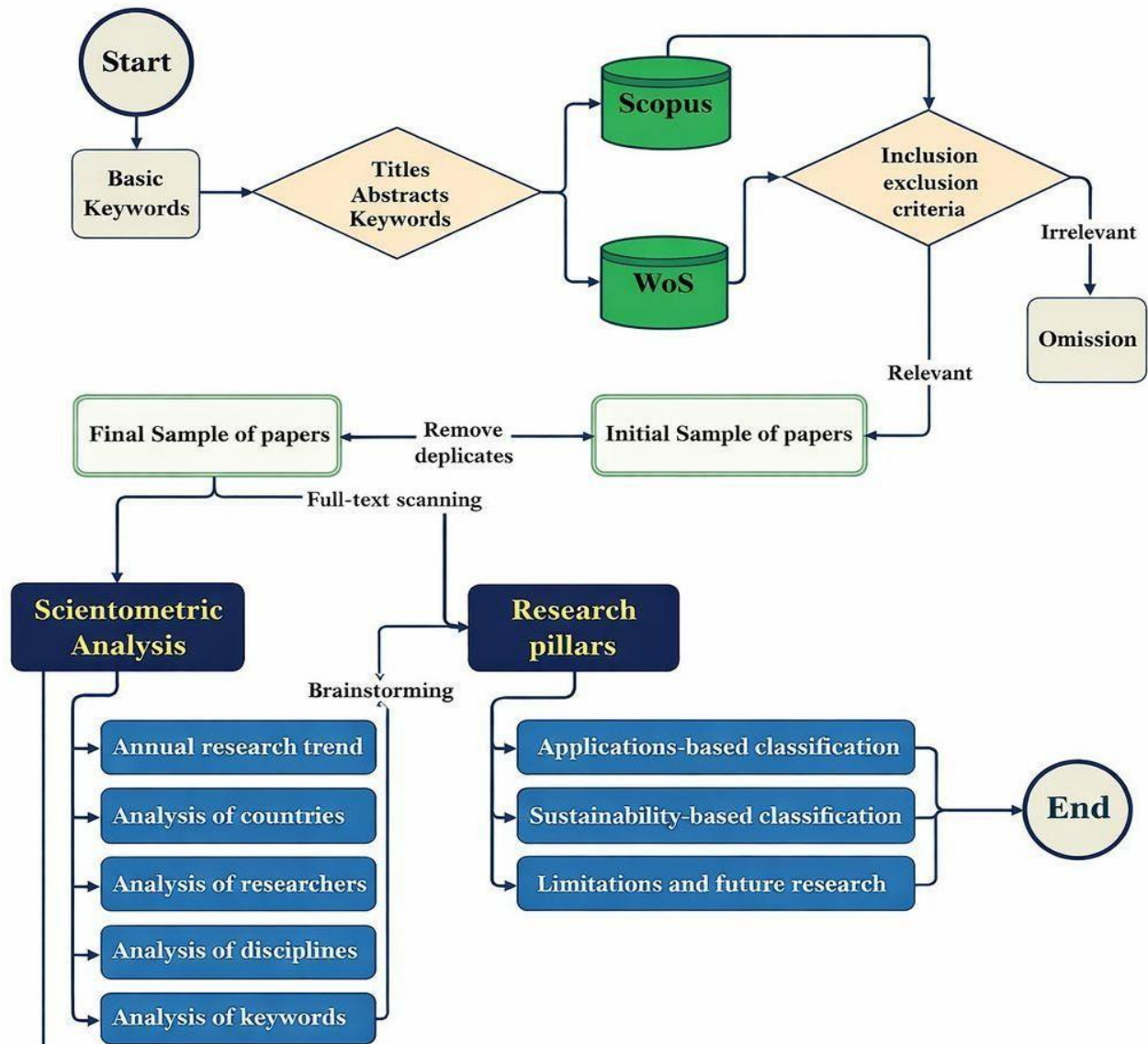
3. Methodology:

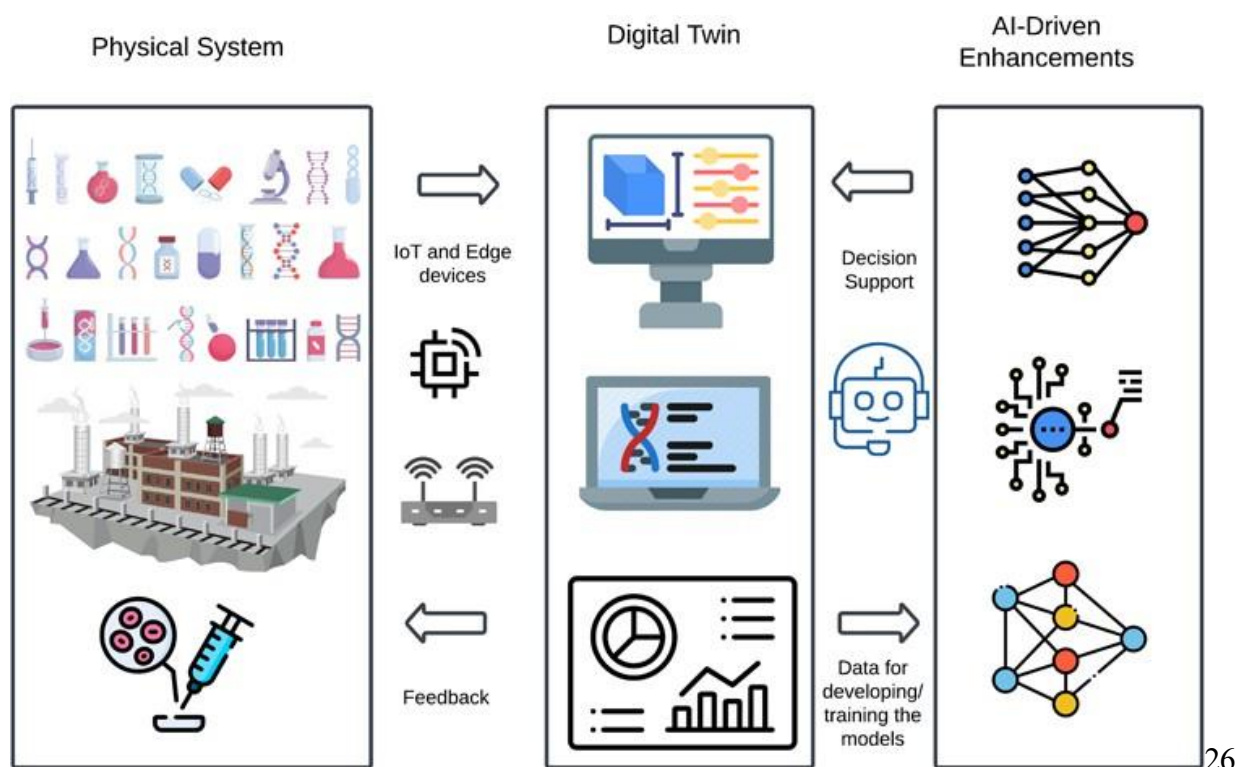
The methodology is divided into two main branches: the scientometric analysis and the identification of research pillars. The scientometric analysis involves examining annual research trends, country-specific contributions, leading researchers, the involvement of various disciplines, and keyword frequency.¹⁸

This analysis provides a quantitative view of the research landscape. Simultaneously, the research pillars are developed through brainstorming and focus on applications-based classification, sustainability-based classification and the identification of limitations and directions for future research.¹⁹

Together, these two branches guide a comprehensive understanding of the research domain, contributing to the development of insights into current trends, knowledge gaps, and future research opportu.²⁰

This study combines quantitative scientometric analysis by evaluating metrics like publication growth, citation patterns, and keyword trends with qualitative analysis of influential studies to interpret emerging themes, research gaps,²¹ and interdisciplinary connections. By integrating both approaches,²² it provides a holistic view of the field, linking statistical trends to contextual insights.^{23,24,25}





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3. Key applications DruG

DTs, which are computer models of organs or cell systems, let scientists test speeds up finding targets, discovering hits, designing molecules, and predicting how drugs behave in the body.²⁷ Generative models can come up with new structures and improve their properties safety and effectiveness virtually, which could cut down **g discovery & preclinical research***²⁸

AI on animal testing. Recent studies show that using AI with traditional models leads to faster development of drug candidates and better predictions before clinical trials.²⁹

1.1 Clinical development & trials (virtual patients, control arms)

Digital patient twins can show how diseases progress and how patients might respond to treatments.³⁰ They help plan studies,³¹ cut down on the need for real placebo groups, and run virtual trials to support or make real trials safer. Regulators and companies are looking into these tools right now.³²

1.2 Manufacturing, quality, and supply chain*

Digital twins that use real-time sensor and PAT data can predict when equipment might fail, help optimize processes as they happen, and ensure product quality throughout production.³³ This helps avoid failed batches and makes production faster. More companies in the pharmaceutical industry are starting to use this technology.³⁴

1.3 Personalized medicine and clinical decision support

Patient-specific digital twins, which combine data like genetics, imaging, electronic health records³⁵, and drug models, can help tailor treatments to individual patients, choose the best treatment plans,³⁶ and find new biomarkers. Some early examples, like testing heart devices or simulating cancer responses, have already been used in clinical settings³⁷

2. Technical approaches & architectures

Hybrid modeling: Combines traditional models like pharmacokinetic or pharmacodynamic models,

which are based on biology, with machine learning. This mix makes results easier to understand and helps apply findings to new situations. Generative AI: Can be used to expand data sets, create realistic virtual patients, and design new drug candidates.⁴ But it's important to check the results carefully to make sure they're accurate³⁸. Data integration and streaming: Digital twins need constant data from sensors during manufacturing or from medical records and lab tests for patient twins. Special software helps keep all this data in sync, adjust for errors, and handle uncertainty.³⁹⁶

3. Regulatory, validation & ethical landscape

Regulators like the FDA, EMA, and MHRA are paying more attention to how AI and digital tools are used. Recent reports and guidelines highlight the need for clear information, proper testing,⁴⁰ consistent results, managing risks, and making sure people are involved in decision-making. Using virtual control groups or data from digital tools needs a clear plan for checking their accuracy and talking through the details with regulators. Privacy, getting permission, and avoiding bias in models are big ethical issues.⁴¹¹³

4. Main benefits observed

- Faster candidate selection and iteration in discovery.
- Reduced costs and time for process optimization and fewer failed batches in manufacturing.
- More efficient clinical trial design (fewer amendments, better enrichment).²¹
- Potential to reduce animal testing and enable personalized dosing⁴²

5. Challenges & limitations

Data quality & interoperability: * heterogeneous, siloed data (EHRs, omics, PAT) hamper building robust DTs.⁴³

6. Conclusion

AI and digital twins together form a powerful, complementary toolkit for pharmaceutical R&D and operations.⁴⁴ They promise efficiency gains, safer products, and more personalized care, but robust data infrastructure, rigorous validation, clear regulatory interaction, and ethical safeguards are essential before broad clinical or regulatory substitution of physical experiments or trials is feasible.⁴⁵

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