e-ISSN: 2320-4230, p-ISSN: 2961-6085

Journal of Drug Discovery and Therapeutics

Available Online at www.jddt.in

CODEN: - JDDTBP (Source: - American Chemical Society)

Volume 14, Issue 5; 2026, 1-9

Artificial Intelligence in Pharmaceutical Manufacturing: Applications, Evidence Maturity, Manufacturing Impact, and GMP-Ready Implementation

Digvijay Singh Rathore[1], Hemant Kumar Kuldeep[2] , Dr. Pawan Kumar Basniwal[3]

[1]Scholar, Sri Balaji College of Pharmacy, Jaipur, Rajasthan, India
[2]Assistant Professor, Sri Balaji College of Pharmacy, Jaipur, Rajasthan, India
[3]Professor & Principal, Sri Balaji College of Pharmacy, Jaipur, Rajasthan, India

Received: 07-08-2026/ Revised: 27-08-2026/ Accepted: 05-09-2026
***Corresponding author: Digvijay Singh Rathore**
Conflict of interest: No conflict of interest.

Abstract:

Artificial intelligence (AI) is increasingly being investigated as a component of smart pharmaceutical manufacturing through machine learning (ML), artificial neural networks (ANNs), deep learning, computer vision, process analytical technology (PAT), predictive maintenance, and digital twins. The underlying review report identified applications across API synthesis, crystallization, blending, granulation, drying, tableting, coating, quality control, inspection, packaging, continuous manufacturing, scheduling, and supply-chain planning. A central limitation of the current literature is that model performance is often emphasized more than manufacturing readiness. High predictive accuracy alone does not establish suitability for a GMP environment because data quality, representativeness, robustness, interoperability, validation, explainability, cybersecurity, human oversight, and lifecycle management also determine practical readiness. This review therefore evaluates AI using an evidence-maturity perspective distinguishing conceptual research, laboratory proof-of-concept, pilot/production-relevant evidence, and routine industrial implementation. It synthesizes implementation barriers and proposes an integrated adoption pathway linking manufacturing-problem definition, data readiness, AI selection, model development, risk-based GMP assessment, pilot testing, industrial integration, and continuous monitoring. The review concludes that the next phase of pharmaceutical AI should focus less on isolated high-performing models and more on validated, trustworthy, integrated, and lifecycle-managed systems that improve quality, productivity, reliability, and patient safety.

Keywords: Artificial intelligence; machine learning; pharmaceutical manufacturing; process analytical technology; digital twins; predictive maintenance; Pharma 4.0; GMP; model validation; manufacturing readines

1. Introduction

Pharmaceutical manufacturing is a highly regulated and data-intensive activity in which raw materials, process parameters, equipment performance, environmental conditions, and product quality attributes must be controlled consistently. Conventional manufacturing remains dependent on predefined operating conditions, periodic sampling, laboratory testing, manual inspection, and established

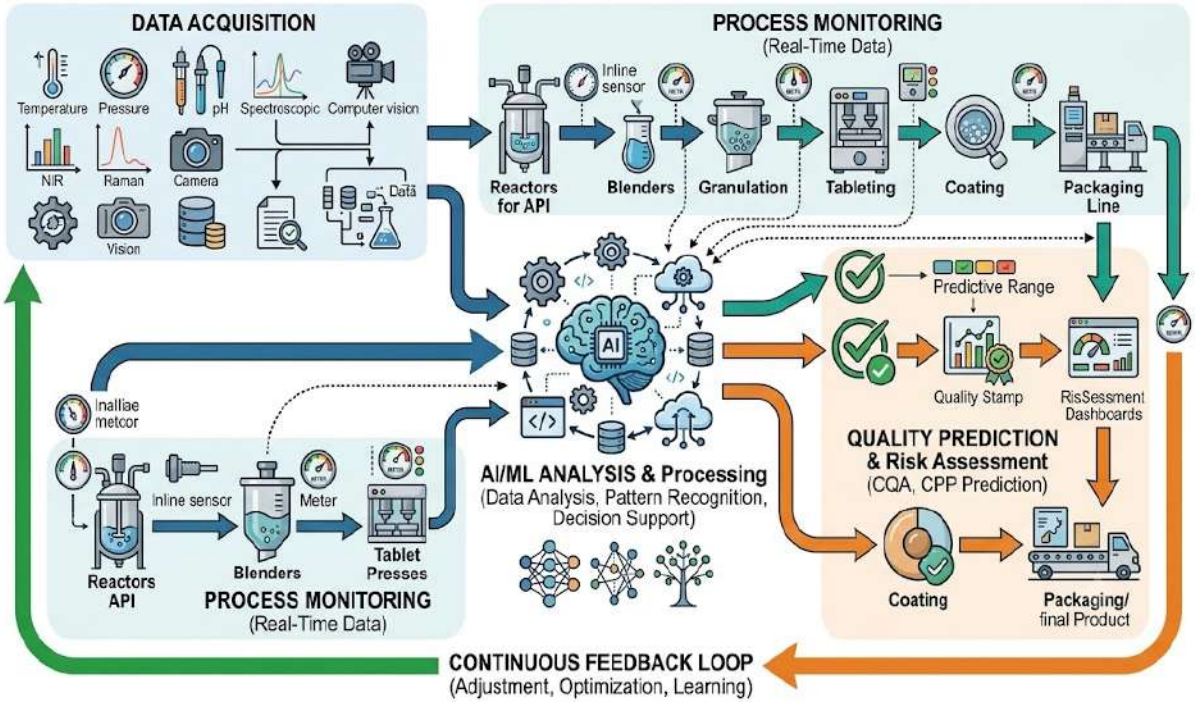
process-control strategies. Increasing availability of sensor, laboratory, manufacturing-execution, and process-control data creates opportunities to complement these approaches with data-driven prediction and decision support.

AI broadly refers to computational approaches capable of learning, pattern recognition, prediction, optimization, reasoning, or decision support, while ML enables models to learn relationships from data rather than relying only on explicitly programmed rules. Industry 4.0 and Pharma 4.0 have strengthened the relevance of AI by connecting sensors, automation, PAT, manufacturing systems, advanced analytics, robotics, and digital twins.

The historical development relevant to pharmaceutical science includes Turing's work on machine intelligence, the Dartmouth proposal and workshop, computational chemistry and QSAR, DENDRAL and expert systems, followed by statistical learning and neural networks. In manufacturing, computerized process control, Quality by Design (QbD), PAT, Industry 4.0, IoT, and digital twins created the infrastructure in which modern AI can operate. The resulting information pathway can be represented as sensor → data → model → prediction → decision → process control.

The underlying report identified five gaps: manufacturing is often treated as only one part of the wider pharmaceutical AI landscape; applications are commonly discussed separately rather than as an integrated ecosystem; evidence maturity is insufficiently differentiated; technical performance receives more attention than GMP implementation; and data, skills, legacy equipment, cybersecurity, cost, and organizational barriers are often treated independently. The key question is therefore not simply where AI can be used, but how technically successful AI can become manufacturing-ready and GMP-compatible.

2. AI Technologies and Applications in Pharmaceutical Manufacturing



2.1 Core AI technologies

ML models can learn relationships between manufacturing inputs such as temperature, pressure, mixing speed, moisture, feed rate, and material properties and outputs such as moisture content, particle size, tablet hardness, API concentration, dissolution, or deviation probability. ANNs are particularly useful for nonlinear relationships and have been investigated across synthesis, crystallization, blending, granulation, drying, tableting, product characterization, and PAT. Deep learning extends these capabilities to complex image and time-series data, although higher complexity can increase computational, explainability, and validation requirements.

Computer vision supports automated inspection of tablets, capsules, containers, labels, and packaging. Digital twins provide dynamic digital representations of processes or equipment and can combine sensor information, process data, mechanistic models, historical information, and AI models for simulation, optimization, monitoring, predictive maintenance, and control. Hybrid AI, combining mechanistic knowledge with data-driven learning, is particularly relevant where datasets are limited but scientific process knowledge is strong.

Table 1:

AI technology	Primary role	Representative use
ML / ANN	Prediction; nonlinear modelling	CQA prediction; process optimization
Deep learning / CNN	Pattern and image recognition	Defect and visual inspection
Time-series ML	Dynamic prediction	Process monitoring
Anomaly detection	Deviation identification	Quality/process monitoring
Digital twins	Simulation; system modelling	Optimization; control; maintenance
Hybrid / explainable AI	Mechanistic integration; interpretation	Process understanding; decision support

2.2 Manufacturing applications

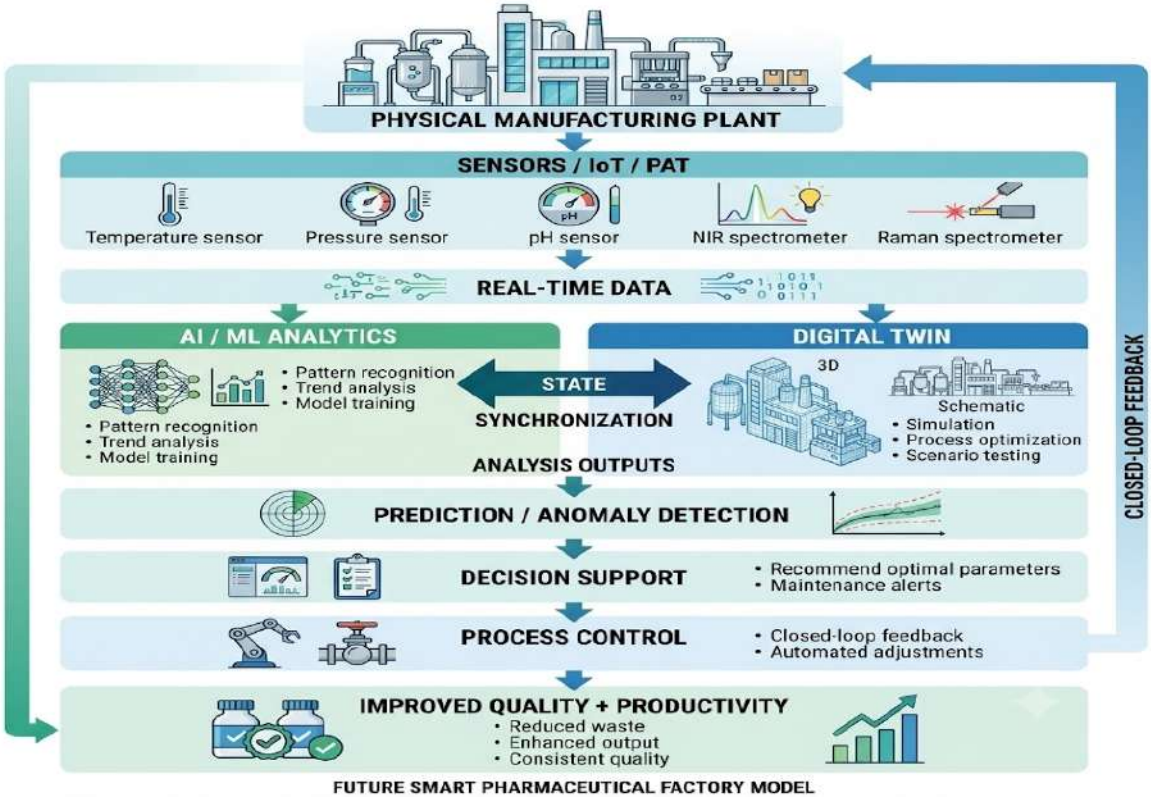
AI is being investigated across the manufacturing chain. In API synthesis, models can relate reaction conditions to yield, selectivity, temperature, time, and reagent concentration, potentially reducing the need to test every experimental condition physically. In crystallization, AI can support prediction of crystal growth, crystal-size distribution, polymorphism-related behaviour, and process endpoints. For blending and granulation, models can relate mixing conditions and material properties to uniformity, moisture, density, flow, and compressibility.

Drying models can predict residual moisture from temperature, airflow, time, and inlet conditions, potentially reducing over- or under-drying. In tableting, AI can model interactions among compression force, dwell time, turret speed, powder properties, density, and porosity to predict hardness, friability, weight variation, tensile strength, capping, and dissolution-related characteristics.

PAT is a major point of convergence between AI and pharmaceutical manufacturing. NIR, Raman, FTIR, imaging, particle-size, temperature, pressure, moisture, and flow measurements generate multivariate data that AI models can translate into predicted quality attributes. However, the report emphasizes that many PAT-AI studies remain at feasibility level, while sustained real-time industrial

implementation is comparatively less common.

AI can support quality control and computer-based inspection by detecting abnormal process trends, product defects, packaging errors, unusual analytical patterns, and parameter deviations. For visual inspection, sensitivity, specificity, false-positive and false-negative rates, robustness, and challenge testing are important. Predictive maintenance can use vibration, temperature, motor current, pressure, equipment history, and maintenance records to anticipate deterioration; rare failures, however, create a major data limitation. Continuous manufacturing is attractive because data are generated continuously, enabling the concept of PAT + AI + continuous manufacturing: continuous sensing → continuous prediction → continuous control. Digital twins extend this concept by connecting physical processes with virtual models. AI also supports packaging inspection, line optimization, demand forecasting, inventory management, scheduling, supplier-risk prediction, raw-material planning, and distribution



FUTURE SMART PHARMACEUTICAL FACTORY MODEL

3. Evidence Maturity: Why Model Accuracy Is Not Enough

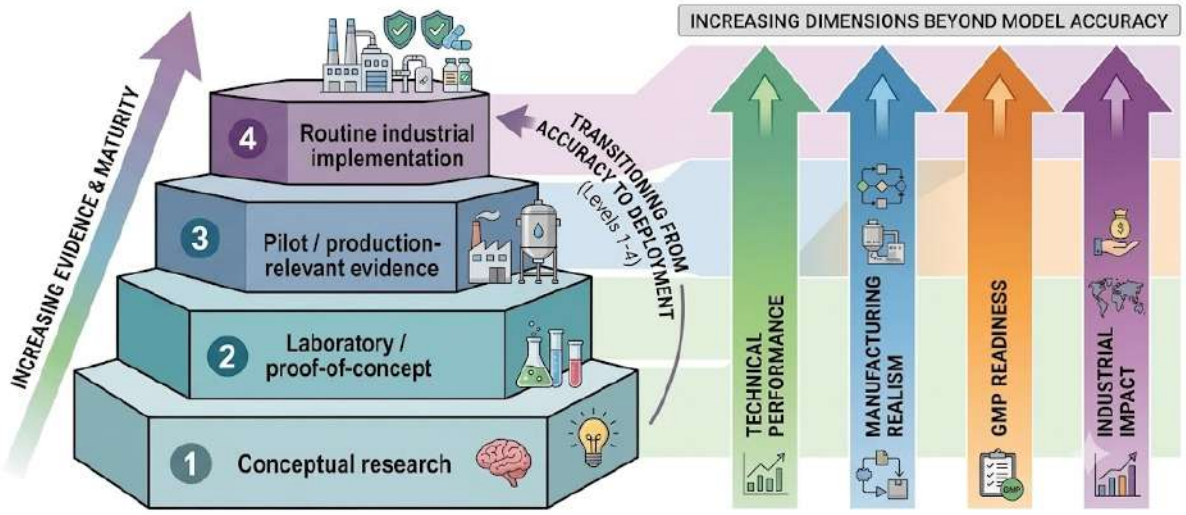
A central contribution of the review is the distinction between AI research performance and manufacturing readiness. A high-performing model developed on a small or controlled dataset may not remain reliable when exposed to raw-material variability, equipment changes, sensor drift, process changes, or new operating conditions. Manufacturing readiness therefore requires multidimensional assessment rather than a single accuracy metric.

Table 2:

Evidence level	Description	Manufacturing significance
Level 1 – Conceptual	Frameworks, proposed architectures, conceptual digital twins	Theoretical potential
Level 2 – Laboratory / proof-of-concept	Controlled experiments, small datasets, simulations	Technical feasibility
Level 3 – Pilot / production-relevant	Pilot scale, commercial equipment, realistic datasets, real-time testing	Practical feasibility
Level 4 – Routine industrial implementation	Routine operation, validated systems, lifecycle control, documented benefits, GMP-compatible use	Manufacturing readiness

The review proposes assessing technical performance together with data quality, manufacturing realism, system integration, GMP readiness, explainability, cybersecurity, lifecycle management, economic value, and workforce readiness. The question therefore changes from 'Is the model accurate?' to 'Is the complete AI system reliable, controllable, validated, useful, and maintainable in the intended manufacturing environment?'

Proposed evidence-maturity framework for evaluating AI applications in pharmaceutical manufacturing beyond model accuracy.



A multidimensional framework for the real-world deployment of AI in regulated pharmaceutical manufacturing.

4. Manufacturing Impact

AI has potential to shift pharmaceutical manufacturing from predominantly reactive responses toward predictive and preventive decision-making. For quality, models may identify process conditions associated with poor quality before final-product release, supporting the conceptual transition from detect → reject toward predict → prevent. Productivity may improve through process optimization, faster troubleshooting, improved scheduling, and predictive maintenance. Waste may be reduced through fewer rejected batches, unnecessary tests,

process variability, over-processing, and unplanned downtime. Equipment reliability may improve through the transition from reactive to preventive and predictive maintenance. These benefits should, however, be demonstrated against a defined manufacturing baseline rather than inferred from model performance alone.

Table 3:

Performance area	Potential AI contribution
Quality	Predictive quality control; earlier deviation detection
Productivity	Process optimization; scheduling
Cost	Waste and downtime reduction
Reliability	Predictive maintenance
Inspection	Automated visual inspection
Decision-making	Real-time analytics; decision support
Continuous manufacturing	Real-time monitoring and control

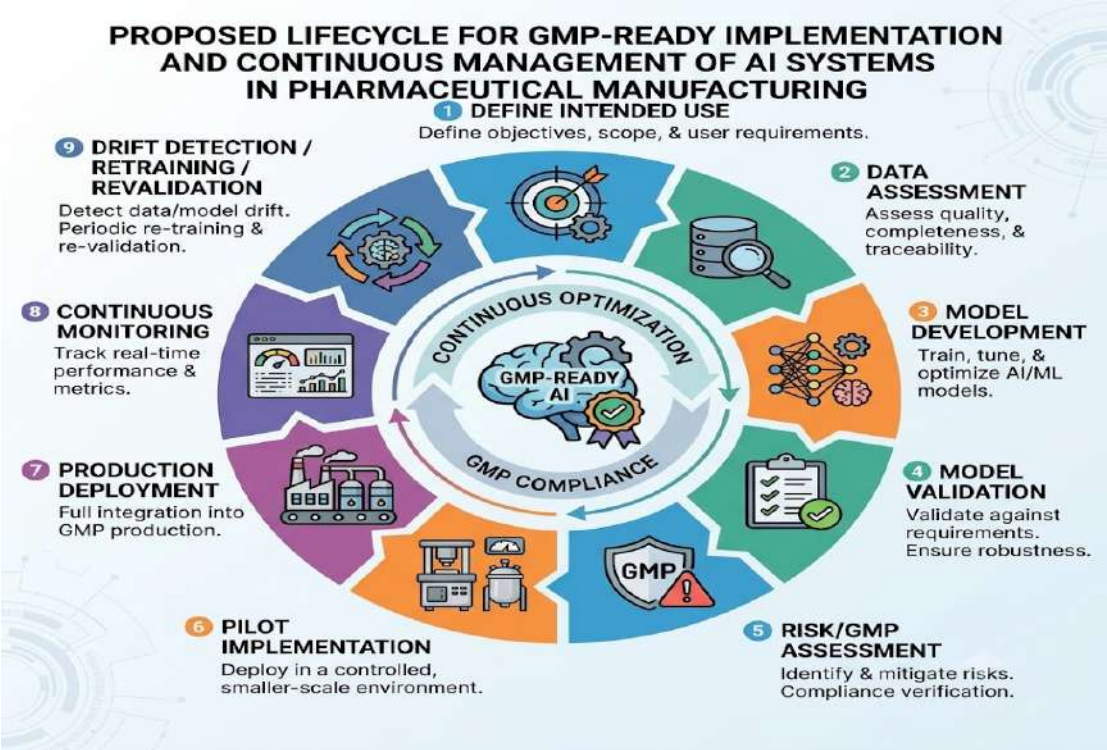
5. Implementation and GMP Considerations

The major barriers identified are data quality and availability, legacy equipment, workforce capability, cost, explainability, cybersecurity, model drift, and regulatory uncertainty. AI requires accurate, complete, representative, correctly labelled, and consistent data. Rare events such as major deviations and equipment failures may have the least training data. Legacy equipment may also lack modern digital interfaces, making interoperability and infrastructure modernization necessary.

Implementation requires multidisciplinary competence spanning pharmaceutical manufacturing, AI, data science, automation, GMP, and validation. Costs may arise from sensors, data infrastructure, software, computing, cybersecurity, validation, and training; consequently, projects should have a clear business case. Explainability becomes particularly important when model outputs influence quality decisions, while connected systems require cybersecurity controls against unauthorized access, data manipulation, malicious inputs, and system disruption.

Model drift is a lifecycle concern because changes in raw materials, equipment, maintenance, formulation, environment, or sensors can alter model performance. A suitable lifecycle is development → validation → deployment → monitoring → change control → retraining → revalidation → retirement. In GMP environments, AI should be controlled, validated, documented, traceable, and monitored, with controls proportionate to intended use and risk.

Risk-based validation is especially important. An AI system used only to visualize trends is lower risk than one predicting equipment failure, while an AI system influencing a critical process parameter or quality decision is higher risk. Validation should consider accuracy, precision, robustness, independent testing, uncertainty, failure modes, operating range, and input quality. Data integrity must extend across collection, storage, processing, model training, prediction, reporting, and archival. For high-risk uses, human oversight remains essential: AI prediction + human expertise + GMP controls should form the controlled decision process rather than treating an AI output as an automatic decision.



6. Integrated AI-Adoption Framework and Future Directions

The review proposes an eight-stage adoption pathway: (1) define the manufacturing problem; (2) assess data readiness; (3) select AI technology according to the problem; (4) develop the model using training, validation, and independent test data; (5) perform risk and GMP assessment; (6) conduct a pilot under realistic manufacturing conditions; (7) integrate the validated system with PAT, sensors, manufacturing-execution systems, equipment, and quality systems; and (8) continuously monitor performance, detect drift, investigate changes, update under change control, and revalidate when required.

Future research should move beyond isolated unit operations toward integrated AI across granulation → drying → compression → coating → quality. Real-time PAT-AI deployment, online validation, model-drift management, digital twins spanning multiple unit operations, hybrid mechanistic/data-driven models, explainable AI, regulatory science, and transparent economic evaluation are particularly important. The future pharmaceutical factory can be conceptualized as a closed information loop: raw materials → sensors/IoT → PAT → real-time data → AI/ML → prediction and anomaly detection → digital twin → decision support → human/automated control → manufacturing → quality attributes → continuous feedback. The central operating principle is Sense → Analyse → Predict → Decide → Act → Learn.

7. Conclusion

AI is becoming an important component of the transition toward intelligent pharmaceutical manufacturing. The reviewed evidence supports applications in process optimization, PAT, API synthesis, crystallization, blending, granulation, drying, tableting, quality control, computer

vision, predictive maintenance, continuous manufacturing, digital twins, packaging, scheduling, and supply-chain planning. Nevertheless, the evidence is heterogeneous, and a substantial proportion remains conceptual, laboratory-based, or proof-of-concept. Real-time deployment, multi-unit-operation integration, long-term performance, and routine GMP implementation remain less mature.

The principal challenge is not simply developing more accurate algorithms, but developing trustworthy AI systems that can operate within pharmaceutical quality systems. The proposed evidence-maturity framework and integrated adoption pathway emphasize that data quality, manufacturing realism, interoperability, validation, explainability, cybersecurity, lifecycle management, economics, and workforce readiness must accompany technical performance. The most credible future direction is an integrated architecture combining AI, PAT, IoT, digital twins, advanced process control, human expertise, and GMP to improve pharmaceutical quality, efficiency, reliability, flexibility, and patient safety.

References

1. Turing, A. M. (1950). Computing machinery and intelligence. Mind, 59(236), 433–460. https://doi.org/10.1093/mind/LIX.236.433
2. U.S. Food and Drug Administration. (2004). PAT—A framework for innovative pharmaceutical development, manufacturing, and quality assurance: Guidance for industry.
3. International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use. (2009). ICH Q8(R2): Pharmaceutical development.
4. International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use. (2008). ICH Q9: Quality risk management.
5. International Council for Harmonisation of Technical Requirements for Pharmaceuticals for Human Use. (2023). ICH Q10: Pharmaceutical quality system.
6. Mastrantonas, A., et al. (2024). The impact of Industry 4.0 on sustainability and sustainable development goals in the pharmaceutical industry. Discover Sustainability, 5, 460. https://doi.org/10.1007/s43621-024-00716-2
7. Kulkov, I. (2021). The role of artificial intelligence in business transformation: A case of pharmaceutical companies. Technology in Society, 66, 101629. https://doi.org/10.1016/j.techsoc.2021.101629
8. Selvaraj, C., Chandra, I., & Singh, S. K. (2022). Artificial intelligence and machine learning approaches for drug design: challenges and opportunities for the pharmaceutical industries. Molecular Diversity, 26, 1893–1913. https://doi.org/10.1007/s11030-021-10326-z
9. Koul, P., & Koul, I. B. (2025). Applications of artificial intelligence and robotics in pharmaceutical sciences: Advancing drug discovery, personalized medicine, and pharmaceutical manufacturing. Tropical Journal of Pharmaceutical and Life Sciences, 12(2), 1–21. https://doi.org/10.61280/tjpls.v12i2.169
10. Nizamuddin, S. F. S., Ikramuddin, M., & Dhore, N. S. (2025). Artificial intelligence in pharmaceutical sciences: Transforming drug discovery, formulation, and manufacturing. Mediterranean Journal of Medical Research, 2(4), 269–275.

https://doi.org/10.5281/zenodo.17945149

11. Page, M. J., McKenzie, J. E., Bossuyt, P. M., et al. (2021). The PRISMA 2020 statement: An updated guideline for reporting systematic reviews. BMJ, 372, n71. https://doi.org/10.1136/bmj.n71
12. Kolluri, S., Lin, J., Liu, R., Zhang, Y., & Zhang, W. (2022). Machine learning and artificial intelligence in pharmaceutical research and development: A review. The AAPS Journal, 24, 19. https://doi.org/10.1208/s12248-021-00644-3
13. Saini, J. P. S., Thakur, A., & Yadav, D. (2025). AI-driven innovations in pharmaceuticals: optimizing drug discovery and industry operations. RSC Pharmaceutics, 2, 437–454. https://doi.org/10.1039/D4PM00323C
14. Okwudiri, N. O., Nwafor, A. E., & Umetiti, C. B. (2025). Harnessing artificial intelligence for improved quality assurance in the pharmaceutical sector: Opportunities and barriers. African Journal of Advances in Sciences and Technology Research, 19(1), 201. https://doi.org/10.62154/ajastr.2025.019.01022
15. Rajesh, M. V., & Elumalai, K. (2025). The transformative power of artificial intelligence in pharmaceutical manufacturing. Journal of Holistic Integrative Pharmacy, 6, 125–135. https://doi.org/10.1016/j.jhip.2025.03.007
16. Manchadi, O., Ben-Bouazza, F.-E., Edder, A., Tafala, I., & Jioudi, B. (2025/2026). Predictive maintenance in pharma manufacturing: Challenges and strategic directions. Engineering Proceedings, 112, 80. https://doi.org/10.3390/engproc2025112080
17. Pazhayattil, A. B., & Konyu-Fogel, G. (2023). An empirical study to accelerate machine learning and artificial intelligence adoption in pharmaceutical manufacturing organizations. Journal of Generic Medicines, 19(2), 81–91. https://doi.org/10.1177/17411343221151109
18. Chen, Y., Yang, O., Sampat, C., Bhalode, P., Ramachandran, R., & Ierapetritou, M. (2020). Digital twins in pharmaceutical and biopharmaceutical manufacturing: A literature review. Processes, 8(9), 1088. https://doi.org/10.3390/pr8091088
19. Abbas, K., Afaq, M., Khan, T. A., & Song, W.-C. (2020). A blockchain and machine learning-based drug supply chain management and recommendation system for smart pharmaceutical industry. Electronics, 9, 852. https://doi.org/10.3390/electronics9050852
20. Al-Hourani, S., & Weraikat, D. (2025). A systematic review of artificial intelligence (AI) and machine learning (ML) in pharmaceutical supply chain resilience: Current trends and future directions. Sustainability, 17, 6591. https://doi.org/10.3390/su17146591