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Review Article

Artificial Intelligence and Machine Learning in Drug Discovery and Pharmacy Practice: An Indian Perspective

Deshmukh Aarati*, Vidya Salunkhe, Ashwini Kamble

Shri Ganpati Institute of Pharmaceutical Sciences and Research Tembhurni.

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ABSTRACT

Artificial intelligence (AI) and machine learning (ML) are increasingly being incorporated into pharmaceutical research, drug discovery and pharmacy practice. Conventional drug development is constrained by complex biology, large experimental workloads, lengthy development pathways, high expenditure and substantial attrition between discovery and clinical approval. AI/ML methods can analyse chemical, biological, clinical and literature-derived data to support target identification, virtual screening, molecular property prediction, de novo molecular design, lead optimisation, ADMET prediction, drug repurposing and clinical-development activities. In pharmacy practice, AI can support medication review, drug–drug interaction detection, medication-error identification, pharmacovigilance, clinical decision support, medication reconciliation and patient-facing digital services. Recent evidence also indicates a rapidly expanding role for AI in clinical pharmacy workflows, although most applications remain decision-support tools rather than autonomous clinical systems. [1–6] The Indian context is especially important because India combines a major pharmaceutical manufacturing base with expanding biomedical research, digital-health infrastructure and government-supported pharmaceutical R&D. The Department of Pharmaceuticals has established the PRIP scheme to promote research and innovation in the Pharma MedTech sector, while the Indian Council of Medical Research (ICMR) has issued dedicated ethical guidance for AI in biomedical research and healthcare. A recent survey of Indian pharmacologists found that 68.26% of respondents were familiar with AI/ML/deep learning, while major concerns included algorithmic bias, skill loss, job displacement and data security. [7–10] This review critically examines the opportunities, evidence, limitations, ethical considerations, regulatory context and future directions for responsible AI adoption in Indian pharmacy and pharmaceutical science.

***Corresponding Author:** Deshmukh Aarati
Address: Shri Ganpati Institute of Pharmaceutical Sciences and Research Tembhurni
Email ✉: deshmukhaarti2705@gmail.com

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INTRODUCTION

Drug discovery is a multidisciplinary process involving disease-mechanism understanding, target identification and validation, hit identification, lead optimisation, preclinical testing, clinical trials, regulatory evaluation and post-marketing surveillance. Traditional discovery remains essential but is resource-intensive and increasingly data-heavy. Recent literature describes AI/ML as complementary technologies that can help researchers prioritise hypotheses, analyse complex datasets and reduce computational bottlenecks across multiple stages of the discovery pipeline. [1,2]

AI is a broad field encompassing computational systems capable of performing tasks associated with learning, reasoning, prediction or pattern recognition. ML is a subset of AI in which algorithms learn relationships from data. Deep learning uses multilayer neural networks, while newer approaches include graph neural networks (GNNs), transformers, diffusion models, foundation models and generative AI. Their value in pharmaceutical research depends not only on model architecture but also on data quality, endpoint definition, external validation and integration with experimental science. [1,2]

The current literature increasingly emphasises a human –AI partnership rather than complete automation. Recent critical reviews describe successful examples of AI-assisted repurposing and molecular discovery but also document clinical-development failures, demonstrating that computational acceleration does not guarantee therapeutic success. [2] Therefore, AI should be regarded as an enabling technology whose outputs require chemical, biological, clinical and regulatory interpretation.

2. Objectives of the Review

- To describe major AI and ML applications across the pharmaceutical drug-discovery pipeline.
- To examine current applications of AI in community, hospital and clinical pharmacy practice.
- To evaluate the Indian research, policy and workforce context for AI adoption.
- To discuss data quality, bias, interpretability, privacy, validation and regulatory challenges.
- To identify the implications of AI for B. Pharm education and the future professional role of pharmacists.
- To propose practical principles for responsible, pharmacist-centred implementation.

3. Review Methodology

This manuscript is a narrative, research-based review rather than a systematic review or meta-analysis. The literature was identified using PubMed/PMC, ScienceDirect, official Government of India sources, ICMR and WHO publications, with emphasis on recent literature published through 2026. Search concepts included combinations of artificial intelligence, machine learning, deep learning, generative AI, drug discovery, clinical pharmacy, pharmacovigilance, medication safety, India and pharmaceutical development.

Priority was given to peer-reviewed reviews, primary studies and authoritative policy/guidance documents. Recent evidence from 2025–2026 was preferentially incorporated where relevant, while established guidance from WHO and ICMR was retained for ethics and governance. Because this is not a systematic review, no pooled effect estimates or formal risk-of-bias meta-analysis is claimed. The purpose is to synthesise current evidence and provide an India-focused scholarly overview suitable for educational and manuscript-development use.

4. AI/ML Applications in Drug Discovery

4.1 Target Identification and Validation

AI can integrate genomics, transcriptomics, proteomics, disease phenotypes, pathway information and biomedical literature to prioritise potential therapeutic targets. Natural-language processing can extract relationships among diseases, genes, proteins, drugs and clinical observations from large literature collections. These approaches can accelerate hypothesis generation, but biological causality still requires experimental validation. [1,2]

4.2 Virtual Screening and Hit Identification

Virtual screening uses computational models to rank compounds according to predicted interaction, activity

or drug-like properties. ML can use molecular descriptors, fingerprints, three-dimensional structures and experimentally measured activities. By reducing the number of compounds requiring experimental testing, AI may improve screening efficiency; however, performance can fall when models encounter chemical space that differs from the training data. [1,2]

4.3 Molecular Generation and De Novo Design

Generative AI can propose new molecular structures according to predefined objectives such as predicted potency, selectivity, physicochemical properties and synthetic feasibility. Transformers, diffusion models and other generative architectures have expanded the computational design space. Nevertheless, generated molecules must undergo chemical feasibility assessment, synthesis, in-vitro testing, pharmacokinetic evaluation and safety assessment before therapeutic claims can be made. [1,2]

4.4 Lead Optimisation

Lead optimisation involves balancing potency, selectivity, solubility, permeability, metabolic stability and toxicity. AI can support multi-parameter optimisation by predicting molecular properties and ranking candidate analogues. This is particularly useful when medicinal chemists must evaluate multiple competing objectives simultaneously.

4.5 ADMET and Toxicity Prediction

Prediction of absorption, distribution, metabolism, excretion and toxicity (ADMET) is an important area for early de-risking. AI models can identify candidate compounds with potentially undesirable properties before expensive downstream experiments. However, differences between in-silico predictions, in-vitro assays and human biology require careful validation and should prevent overinterpretation of computational scores.

4.6 Drug Repurposing

AI can integrate drug–target networks, disease mechanisms, biomedical literature and clinical data to identify potential new uses for existing medicines. Repurposing may be attractive because established pharmacological and safety information can provide a starting point. However, a computational association is a hypothesis rather than evidence of clinical efficacy. [2]

4.7 Clinical Development

AI can support patient stratification, trial recruitment, protocol optimisation, endpoint analysis and identification of patterns in clinical data. These applications can improve operational efficiency, but clinical decisions remain dependent on validated evidence and regulatory oversight. AI should not be used to obscure uncertainty or replace appropriate clinical judgement.

Table 1: Major AI/ml Applications Across the Drug-Discovery Pipeline

Stage	Representative AI/ML use	Potential contribution	Main limitation
Target discovery	Omics analysis; NLP; network analysis	Target prioritisation and hypothesis generation	Biological validation and population bias
Hit discovery	Virtual screening; activity prediction	Prioritisation of compounds	Training-data quality and domain shift
Molecule design	Generative AI; transformers; diffusion models	Novel candidate generation	Synthetic feasibility and experimental validation
Lead optimisation	Multi-objective property prediction	Balancing potency and developability	Activity cliffs and uncertain generalisation
ADMET/safety	Predictive modelling	Early liability identification	Human translation and incomplete datasets
Repurposing	Knowledge graphs; network ML	New therapeutic hypotheses	Clinical efficacy not established
Clinical development	Patient stratification; trial analytics	Operational and analytical support	Bias, privacy and regulatory validation

5. AI in Pharmacy Practice

Pharmacy practice generates high-volume information through prescriptions, medication histories, laboratory results, dispensing records, adverse-event reports and clinical documentation. AI can help pharmacists process this information and prioritise cases requiring professional review. A 2023 literature review identified applications in medication management, drug–drug interaction assessment, medicine safety and clinical decision support. [5]

5.1 Medication Review and Clinical Decision Support

AI-enabled systems can flag potentially inappropriate medicines, duplicate therapy, contraindications, dose-related concerns and high-risk combinations. Their greatest value is likely to be prioritisation: the system can identify patients or prescriptions needing closer pharmacist attention, while the pharmacist interprets the clinical context.

5.2 Drug–Drug Interaction Detection

Interaction screening is a mature decision-support application. AI and knowledge-based systems can combine medication lists with patient-specific information to rank potential interactions. The pharmacist must assess whether an interaction is clinically relevant because alerts can be excessive, incomplete or context dependent.

5.3 Medication Error Prevention and Reconciliation

Natural-language processing and predictive models can assist in detecting discrepancies between medication lists, prescriptions and clinical documentation. This may be valuable during admission, transfer and discharge, where incomplete medication histories can contribute to preventable errors.

5.4 Pharmacovigilance

AI can assist adverse-drug-reaction identification from spontaneous reports, clinical notes and other sources. NLP can help extract suspected medicines, symptoms, time relationships and relevant patient characteristics. The approach may increase signal-processing capacity, but human assessment remains necessary to confirm clinical plausibility and causality.

5.5 Patient Counselling and Adherence Support

Conversational systems and digital applications may provide medication reminders, educational information and basic responses to frequently asked questions. In India, multilingual interfaces may increase accessibility. However, automated counselling should not replace pharmacist counselling for complex therapy, vulnerable populations or situations requiring diagnosis and clinical assessment.

5.6 Community Pharmacy and Public Health

Potential community-pharmacy applications include triaging medication-related queries, supporting adherence, identifying repeated high-risk OTC use and assisting referral decisions. Such tools require carefully defined scope so that they do not encourage unsafe self-medication or substitute algorithmic advice for professional assessment.

6. Recent Evidence from Clinical Pharmacy Research

2026 scoping review mapped AI applications in clinical pharmacy services across hospital and community settings. The review searched PubMed, Web of Science and Scopus for literature from 2010–2025 and included 36 publications. Drug-interaction and adverse-drug-effect detection represented 12 studies (33.3%), while medication errors and potentially inappropriate medicines represented 11 studies (30.6%). Machine learning, natural-language processing and deep learning were among the most frequently reported approaches. [6]

These findings are important for pharmacy education because they show that AI is already being studied in pharmacist-facing workflows, but the evidence base remains heterogeneous. Future studies should evaluate clinical outcomes, workflow impact, false-alert rates, external validation and patient safety rather than reporting model accuracy alone.

7. Indian Perspective

India offers a distinctive setting for AI-enabled pharmaceutical research because of its pharmaceutical

manufacturing capacity, generic-drug expertise, biomedical research institutions and expanding digital-health ecosystem. Government policy is also moving toward greater support for pharmaceutical innovation. The Department of Pharmaceuticals currently lists the PRIP scheme as a national programme intended to promote research and innovation in the Pharma MedTech sector. [9]

The Indian workforce perspective is equally important. A 2025 survey of 104 Indian pharmacologists reported that 68.26% were familiar with AI/ML/deep learning. Awareness was higher among industry respondents (82.5%) than academic respondents (59.37%). Respondents also identified algorithmic bias, skill loss, job displacement and data-security issues as important concerns. The study reported that 77% recognised AI's role in drug discovery, 73.07% in pharmacovigilance and 69.23% in clinical trials. [7]

These findings should not be generalised to all Indian pharmacists because the sample was limited to pharmacologists. Nevertheless, they demonstrate a clear need for structured AI literacy across pharmacy education and pharmaceutical workplaces.

8. Implications for B. Pharm Education

AI literacy should become an applied component of modern pharmacy education. Students do not need to become professional programmers, but they should understand how datasets are generated, how models are trained and validated, how bias can occur, and how to interpret model outputs critically.

- Fundamentals of AI, ML, deep learning and generative AI.
- Basic concepts of datasets, training/validation/test sets and external validation.
- Interpretation of sensitivity, specificity, accuracy, precision, recall and calibration.
- Drug-information searching and critical appraisal of AI-generated answers.
- Pharmacovigilance and medication-safety applications of NLP and ML.
- Ethical use of patient data, privacy, consent and governance.
- Recognition of hallucinations, unsupported claims and fabricated references from generative AI.

9. Ethical, Legal and Governance Considerations

9.1 Human Oversight and Accountability

ICMR's 2023 ethical guidelines provide a framework for ethical decision-making in AI-based biomedical research and healthcare, including ethical principles, governance, ethics review and informed consent. [10] AI outputs should therefore be treated as decision-support information when used in patient-care contexts unless a specific system has undergone appropriate validation and authorisation.

9.2 Transparency and Explainability

A model's performance should not be reported only as a single accuracy value. Researchers should describe the intended use, population, input data, outcome definition, validation strategy, known limitations and uncertainty. Explainability is particularly important when AI outputs influence medicine selection or patient safety.

9.3 Data Privacy and Security

Pharmaceutical and clinical datasets may contain sensitive personal information. Data minimisation, de-identification, secure access, controlled sharing and institutional governance are essential. AI systems should be evaluated for risks created by inappropriate data reuse, model leakage or unauthorised access.

9.4 Bias and Equity

AI models can reproduce or amplify biases present in their training data. Models trained predominantly on one population may perform differently in another population. For India, attention is required for demographic diversity, language, healthcare access, socioeconomic variation and differences between tertiary-care and resource-constrained settings.

9.5 Regulatory Considerations

Regulatory expectations for AI-enabled healthcare technologies continue to evolve. In India, CDSCO has issued guidance activity relating to Medical Device Software under the Medical Devices Rules, 2017, illustrating the growing need to address software-

specific regulatory requirements. [11] The exact regulatory pathway depends on the intended use and classification of a product; therefore, an academic review should not imply that all AI systems are regulated identically.

10. WHO Principles for Responsible AI in Health

WHO has emphasised that AI for health should be developed and deployed with ethics and human rights at its centre. Its guidance identifies principles including protection of human autonomy, promotion of well-being and safety, transparency and explainability, responsibility and accountability, inclusiveness and equity, and responsiveness and sustainability. [12]

WHO's 2024 discussion paper on AI in pharmaceutical development and delivery further notes that AI is already being used across many steps of pharmaceutical development and that future use is likely to expand. The document stresses that commercial benefits should be accompanied by public-health benefits and appropriate governance. [13]

In 2025, WHO also issued guidance on large multimodal models, noting their potential use in healthcare, scientific research, public health and drug development while highlighting the need for responsible governance. [14]

11. Potential Benefits

- Faster prioritisation of therapeutic targets and candidate molecules.
- Reduction in the number of low-priority compounds requiring experimental screening.
- Earlier identification of some pharmacokinetic, toxicity and developability liabilities.
- Integration of heterogeneous chemical, biological, clinical and literature data.
- Support for drug repurpose and precision-medicine hypotheses.
- Improved prioritisation of medication-related problems in pharmacy workflows.
- Potential support for pharmacovigilance signal detection and medication safety.
- Greater scalability of data-intensive pharmaceutical research.

12. Limitations and Challenges

12.1 Data Quality

AI systems are highly dependent on the quality, completeness and representativeness of training data. Inconsistent experimental protocols, missing values, duplicate records and biased datasets can produce misleading outputs.

12.2 Generalisability

Strong performance on a retrospective dataset does not guarantee performance in a different hospital, population, chemical space or clinical setting. External validation is therefore essential.

12.3 Interpretability

Complex models may be difficult to explain to clinicians, pharmacists and regulators. This becomes particularly important when outputs influence patient safety.

12.4 False Alerts and Automation Bias

AI systems can generate false-positive or false-negative alerts. Users may also place excessive trust in automated recommendations. Human review and clear escalation pathways are therefore required.

12.5 Cost and Infrastructure

Advanced AI may require specialised computational infrastructure, secure data systems and trained personnel. Unequal infrastructure could widen rather than reduce healthcare disparities.

12.6 Workforce Impact

AI may change job roles and required skills. The appropriate response is workforce development and interdisciplinary training rather than assuming that AI will simply replace professionals.

13. Future Directions

The future of pharmaceutical AI is likely to involve multimodal models that integrate molecular structures, omics data, literature, clinical records and real-world evidence. Foundation models, generative AI, diffusion models, autonomous research agents and automated synthesis platforms may increasingly interact with

conventional computational chemistry and experimental workflows. [1,2,14]

For India, future research priorities should include development of representative Indian datasets, multilingual clinical tools, standardised evaluation frameworks, pharmacist-focused AI curricula, academic–industry partnerships and outcome-based implementation studies. AI projects should move beyond proof-of-concept accuracy toward clinically meaningful endpoints such as medication-error reduction, adverse-event prevention, time saved per medication review, patient outcomes and cost-effectiveness.

A particularly promising model is the 'human-in-the-loop' approach. In this framework, AI performs high-volume data processing and prioritisation, while pharmacists, clinicians, medicinal chemists and regulatory experts retain responsibility for interpretation and decisions. Such collaboration combines computational scale with professional judgement.

Table 2: Practical Framework for Responsible AI Adoption in Pharmacy

Domain	Recommended approach	Expected benefit
Clinical safety	Human review of consequential AI outputs	Reduced risk of unsafe automation
Data governance	Validated, representative and appropriately governed datasets	Improved reliability and equity
Model validation	Internal + external validation; subgroup performance analysis	Better generalisability
Transparency	Document intended use, uncertainty and limitations	Improved trust and accountability
Privacy	Data minimisation, de-identification and access control	Reduced confidentiality risk
Education	AI literacy and critical appraisal training	Competent future workforce
Monitoring	Post-deployment performance and incident monitoring	Early detection of model drift or harm

14. Illustrative AI-Enabled Drug Discovery Examples

Recent literature illustrates why AI should be evaluated realistically. Baricitinib has been discussed as an example of AI-assisted drug repurposing; halicin has been reported as a preclinical antibiotic-discovery example; DSP-1181 demonstrates that rapid AI-assisted discovery does not guarantee clinical success because the programme was discontinued after Phase I; and ISM001-055/rentosertib has been reported in the context of positive Phase IIa results. [2] These examples support a balanced interpretation: AI may accelerate selected stages, but therapeutic development remains dependent on experimental and clinical evidence.

Such case studies are valuable in B.Pharm education because they demonstrate the difference between AI-generated hypotheses, AI-assisted optimisation, clinical development and regulatory approval. Students should avoid describing a molecule as an 'AI-discovered drug' without specifying the exact role AI played in its development.

15. Research Gaps and Proposed Agenda for India

- Need for externally validated AI models using Indian patient and pharmaceutical datasets.
- Need for standard reporting of dataset provenance, model architecture, performance and uncertainty.
- Need for prospective studies assessing clinical and economic outcomes of AI-supported pharmacy services.
- Need for multilingual AI systems appropriate for Indian healthcare communication.
- Need for pharmacist involvement in AI design, validation, implementation and monitoring.
- Need for curricula that combine pharmacology, pharmaceutics, pharmacy practice, statistics and basic data science.
- Need for governance frameworks that define accountability when AI outputs contribute to clinical decisions.

CONCLUSION

AI and ML are becoming important enabling technologies across pharmaceutical research and pharmacy practice. They can support target identification, virtual screening, molecular generation, lead optimisation, ADMET prediction, repurposing and selected clinical-development tasks. In pharmacy practice, AI can assist medication review, interaction detection, medication safety, pharmacovigilance, reconciliation and digital patient support. Recent clinical-pharmacy evidence confirms growing research activity, although implementation evidence remains heterogeneous. [1–6]

India has an opportunity to develop AI-enabled pharmaceutical research and pharmacy services while building on its strong pharmaceutical sector and growing research ecosystem. Government initiatives such as PRIP and national ethical guidance from ICMR provide important policy foundations. However, responsible implementation requires high-quality data, external validation, transparency, privacy protection, equity, appropriate regulatory oversight and trained professionals. AI should therefore be adopted as a complementary technology that strengthens pharmacist and researcher capabilities rather than replacing professional responsibility.

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