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ARTIFICIAL INTELLIGENCE IN PHARMACY: APPLICATIONS, OPPORTUNITIES AND CHALLENGES

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Abstract:

Artificial intelligence (AI) is reshaping every stage of the medicine life cycle, from the identification of drug targets to the counselling of patients at the pharmacy counter. This review examines how AI technologies, chiefly machine learning, deep learning, natural language processing and generative models, are applied across pharmaceutical science and pharmacy practice, and weighs the opportunities they offer against the challenges that limit their safe adoption. In drug discovery, AI supports target identification, protein structure prediction, virtual screening, de novo molecular design, retrosynthesis, drug repurposing and clinical trial optimisation. In pharmaceutics and manufacturing, it is used to predict formulation behaviour, guide three-dimensional printing of dosage forms and enable real-time process control. In clinical, hospital and community pharmacy, AI-enabled tools assist prescription verification, prevention of adverse drug events, dose individualisation, adherence support, inventory management and patient communication. AI also strengthens pharmacovigilance, regulatory science and pharmacy education. The principal opportunities are shorter development timelines, lower attrition, personalised therapy, safer medication use and more efficient operations. The principal challenges are poor data quality and bias, limited transparency of complex models, privacy, unclear accountability, evolving regulation, validation gaps, fabricated output from language models and the need to prepare the pharmacy workforce. We conclude that AI is best viewed as a decision-support partner that extends, and does not replace, the professional judgement of pharmacists and pharmaceutical scientists, and we outline priorities for responsible implementation.

Keywords: *Artificial intelligence; Machine learning; Deep learning; Drug discovery; Pharmacy practice; Pharmacovigilance; Personalised medicine; Pharmaceutical manufacturing.*

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INTRODUCTION:

Pharmacy is a discipline that spans the science of medicines and the care of the people who use them. It covers the discovery of new molecules, their formulation into stable and effective dosage forms, large-scale manufacture, quality assurance, distribution, dispensing, counselling and the monitoring of safety after a product reaches the market. Each of these steps now generates data on a scale that no individual can interpret unaided: high-throughput screening libraries, genomic and proteomic profiles, electronic health records, sensor streams from production lines, prescription claims and spontaneous adverse event reports. Artificial intelligence (AI), defined broadly as the capacity of a computer system to carry out tasks that normally require human intelligence, such as learning, reasoning, perception and language understanding,[1] offers a way to convert these data into usable knowledge.

Why AI is relevant to pharmacy now

Three developments explain the rapid uptake of AI in health care over the past decade: the availability of very large digital datasets, the falling cost of high-performance computing and major algorithmic advances, especially in deep learning.[2–4] Together they have moved AI from a laboratory curiosity to a working tool in clinical and pharmaceutical settings.

The economics of medicine development add urgency. Published estimates of the capitalised cost of bringing one new drug to market range from roughly USD 1 billion to more than USD 2.5 billion, depending on the method and the period examined.[5,6] Few candidates succeed. An analysis of clinical development programmes found that only about one in ten drugs entering phase I eventually reached approval,[7] and a later review attributed most failures to lack of clinical efficacy, unmanageable toxicity, poor drug-like properties and weak strategic planning.[8] Any technology that improves the selection of targets and molecules, or that predicts failure earlier, therefore carries substantial value.

At the other end of the medicine life cycle, pharmacists work under growing pressure. Ageing populations, polypharmacy, rising prescription volumes and persistent risks of medication error and non-adherence all increase the demand for accurate, timely and personalised pharmaceutical care. AI-enabled tools for verification, interaction screening, inventory control and patient communication are now the subject of overviews written specifically for the profession,[9,10] and broader reviews of AI in clinical practice also describe medication management and decision support as expanding areas.[11]

Evolution and Core Technologies of AI

The idea of machine intelligence was formalised at the Dartmouth workshop of 1956. The first decades produced rule-based "expert systems" that encoded the knowledge of specialists as if-then statements; MYCIN, a 1970s system for advising on antimicrobial therapy, is the best-known medical example.[1] Such systems were costly to maintain and brittle outside their narrow domain, and enthusiasm waned. Statistical machine learning matured in the 1990s and 2000s, but the decisive change came after 2012, when deep neural networks trained on large labelled datasets with graphics processors began to outperform earlier methods in image, speech and language tasks.[14] The transformer architecture introduced in 2017 then made it practical to train very large language models on text,[15] and in 2021 a deep-learning system, AlphaFold, predicted the three-dimensional structures of many proteins at close to experimental accuracy,[16] an advance of direct importance to structure-based drug design.

Large language models (LLMs) have since entered clinical and pharmaceutical conversation. One widely cited evaluation showed that an instruction-tuned LLM could score above the usual pass mark on licensing-examination style medical questions, while also documenting important gaps in reliability and safety.[17] Subsequent reviews describe both the promise and the risks of these models in medicine.[18]

AI is an umbrella term. As shown in Figure 1, machine learning (ML) is a subset of AI in which algorithms learn patterns from data rather than following hand-written rules; deep learning (DL) is a subset of ML that uses many-layered neural networks; and generative AI is a family of DL models that produce new content such as text, images or molecular structures. Table 1 summarises the main techniques and their pharmaceutical uses.

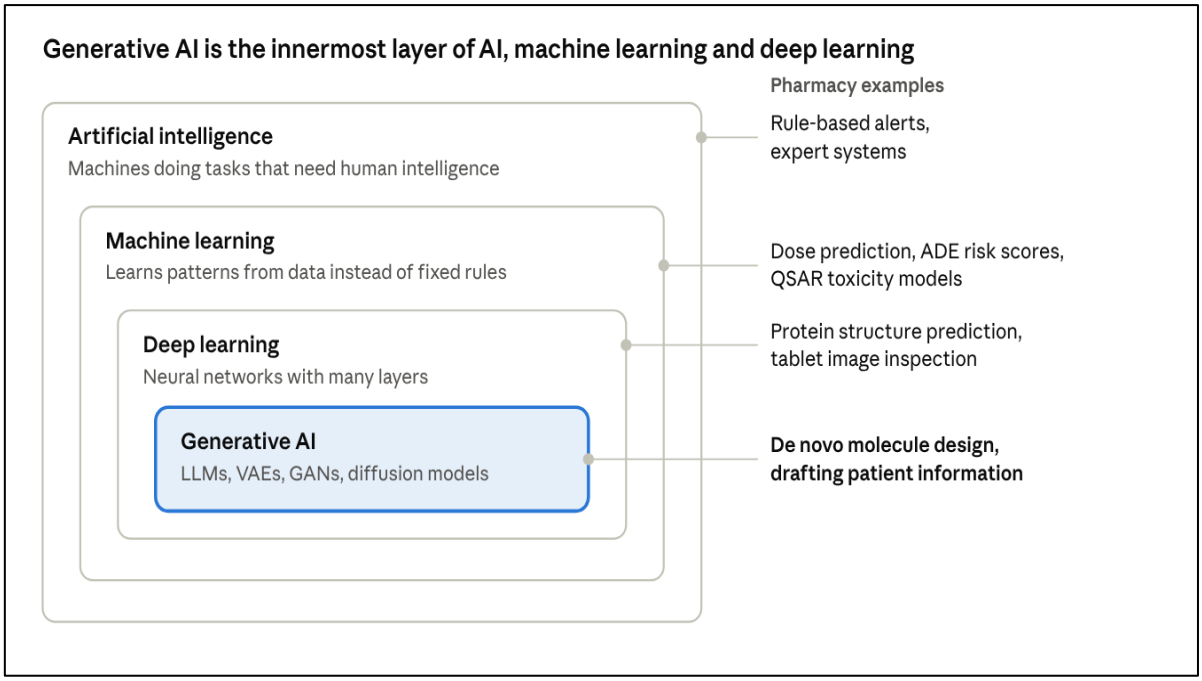


Figure 1. Relationship between artificial intelligence, machine learning, deep learning and generative AI, with examples relevant to pharmacy.

- **Machine learning.** In supervised learning, a model is trained on labelled examples, for instance molecules tagged as toxic or non-toxic, and then predicts labels for new cases. Unsupervised learning looks for structure in unlabelled data, such as groups of patients with similar medication histories. Reinforcement learning improves a sequence of decisions through feedback and has been explored for adaptive dosing and molecular optimisation.[19,20] Common algorithms include logistic regression, random forests, support vector machines and gradient-boosted trees; they work well on structured, tabular data of moderate size.
- **Deep learning.** Deep networks learn their own features from raw input. Convolutional neural networks are suited to images, for example microscopy, histology or tablet inspection; recurrent networks and transformers handle sequences such as text strings that encode molecules; and graph neural networks treat a molecule as a graph of atoms and bonds.[21] Their strength is accuracy on large, complex datasets, and their weakness is a need for substantial data and computing power and a tendency to behave as "black boxes".
- **Natural language processing (NLP).** NLP converts unstructured text into structured information. In pharmacy it is used to read clinical notes, code adverse drug reaction reports, screen the literature and power conversational assistants.[22]
- **Generative models.** Variational autoencoders, generative adversarial networks and diffusion models can propose new molecules with desired properties,[23,24] whereas LLMs generate text, summaries and code.[17,18]
- **Explainable AI and automation.** Explainability methods highlight which inputs drove a prediction and are increasingly demanded by clinicians and regulators.[25] Robotics and laboratory automation, guided by algorithms that select the most informative next experiment (active learning), allow closed design-make-test cycles in discovery laboratories.[26,27]

Table 1. Major AI techniques and their typical pharmaceutical applications

AI technique	Basic principle	Typical applications in pharmacy and pharmaceutical sciences	Refs.
Supervised machine learning	Learns a mapping from labelled inputs to outputs	QSAR, ADMET and toxicity prediction; adverse drug event risk scoring	19,20
Unsupervised machine learning	Finds structure in unlabelled data	Patient stratification; clustering of compound libraries	19,20
Reinforcement and active learning	Improves decisions through feedback; selects informative experiments	Molecular optimisation; adaptive experimental design	20,27

Deep neural networks (CNN, RNN, GNN)	Multi-layer networks learn hierarchical features	Bioactivity prediction; image analysis; molecular property prediction	14,21
Natural language processing	Extracts meaning from free text	Adverse event coding; clinical note mining; literature surveillance; chatbots	22
Generative models (VAE, GAN, LLM)	Produce new molecules or text	De novo drug design; drafting patient information	17,18,23,24
Explainable AI	Exposes the reasoning behind predictions	Clinician trust; regulatory justification	25
Robotics and automation	Physical systems directed by algorithms	Automated synthesis and screening; dispensing robots	26

The data-to-deployment pathway

Whatever the technique, an AI application follows a common pathway: data are collected and curated; features are engineered or learned; a model is trained; its performance is checked on data it has not seen, ideally from another institution; it is deployed within a workflow; and its behaviour is monitored over time because data and practice patterns drift.

Applications in Drug Discovery and Development

Drug discovery is the area where AI has attracted the most investment and the most publicity. The conventional pipeline moves from target selection through hit identification, lead optimisation, preclinical testing and three phases of clinical trials, with high attrition at every step.[4,20,28]

Target identification and validation

A drug target is typically a protein whose modulation changes the course of a disease. Algorithms can mine genomic, transcriptomic, proteomic and literature data to propose and rank candidate targets, often by building knowledge graphs that link genes, pathways, diseases and compounds.[29] Deep learning applied to multi-omics data helps to separate disease subtypes and to identify biomarkers that predict treatment response.[30] Because many predicted associations are only correlative, experimental confirmation remains essential.

Protein structure prediction and virtual screening

Knowing the three-dimensional shape of a target allows molecules to be docked into its binding site. AlphaFold's accurate structure predictions have widened the set of targets that can be approached by structure-based methods.[16] Virtual screening uses scoring functions, classical machine learning or deep neural networks to rank very large compound libraries so that only the most promising molecules need to be tested in the laboratory.[31] Ligand-based approaches predict activity from the similarity of known actives, and deep learning models can combine both ligand and protein information.[32] Screening campaigns guided by neural networks have identified new antibacterial scaffolds: one model trained on growth-inhibition data predicted activity across a library of more than one hundred million molecules and led to the discovery of halicin, a compound with broad antibacterial activity,[33] and an explainable deep-learning approach later identified a new structural class of antibiotics active against methicillin-resistant *Staphylococcus aureus*.[34]

De novo molecular design and synthesis planning

Instead of searching existing libraries, generative models can design molecules from scratch against a specified profile of potency, selectivity and drug-likeness.[23,24,28] In a frequently cited example, a generative reinforcement-learning platform designed inhibitors of discoidin domain receptor 1 (DDR1) and delivered a validated lead within roughly six weeks of starting the design process.[35] AI is also applied to retrosynthesis, the task of working backwards from a target molecule to available starting materials. A system combining deep neural networks with tree search proposed synthetic routes that experienced chemists rated as comparable to routes taken from the literature, and it did so far faster.[36] Generative design still produces many molecules that are hard to make or that lose activity when tested, which is why human medicinal chemists remain central to the process.[32]

Prediction of ADMET and toxicity

A large share of late-stage failures is traced to poor absorption, distribution, metabolism, excretion or toxicity (ADMET).[8] Quantitative structure-activity and structure-property relationship models built with machine learning predict solubility, permeability, metabolic stability, cardiotoxicity (for example hERG channel blockade) and hepatotoxicity directly from chemical structure, allowing weak candidates to be dropped before synthesis.[21,37] Such models are only as good as the training data, and prediction is least reliable for chemical space that differs from the training set.

Drug repurposing

Repurposing existing drugs for new indications saves time because safety profiles are already known.[38] Network-based methods, knowledge graphs and text-mining tools can scan the literature and databases for unexpected drug-disease links. During the COVID-19 pandemic, an AI-assisted knowledge-graph analysis proposed baricitinib, a Janus kinase inhibitor used in rheumatoid arthritis, as a candidate to limit viral entry and inflammation, and the drug subsequently progressed to clinical evaluation.[39]

Clinical trial design and conduct

Clinical trials are the most expensive stage of development. AI can help in several ways: mining electronic health records to find eligible participants and suitable sites, predicting dropout, selecting enrichment biomarkers, simulating trial outcomes, and monitoring data quality and adherence during the study.[40],[41] Industry assessments also describe AI use in protocol design, endpoint selection and digital monitoring through wearables.[42] Most of these tools remain at an early stage of validation, and prospective evidence that they shorten trials or improve success rates is still limited.

What does the evidence on AI-discovered drugs show?

The number of AI-focused discovery companies and partnerships has grown quickly,[43] and the first systematic analysis of clinical results for AI-discovered molecules reported a higher Phase I success rate (about 80-90%) than historical industry averages (about 40-65%), but a Phase II success rate of about 40%, similar to the industry norm, based on a small number of molecules.[44] These data suggest that AI is good at producing candidates that are safe and well tolerated in early human studies, while the harder question of whether they improve efficacy in patients is still open. The most defensible conclusion at present is that AI can raise the quality of the candidates entering the clinic, but it has not yet been shown to remove the biological uncertainty that causes later failures.

Applications in Pharmaceutical Formulation and Manufacturing

Formulation scientists convert an active substance into a dosage form that is stable, bioavailable, manufacturable and acceptable to patients. Historically this has relied on experience, factorial experimental designs and many iterations at the bench. Because formulation development generates large tables of composition, process settings and measured responses, it is a natural fit for machine learning.[45],[46]

Formulation design and property prediction

Models trained on historical formulation data can predict properties such as solubility, disintegration time, dissolution profile and physical stability from the composition and process variables of a proposed formula.[45] This allows scientists to screen many combinations of excipients computationally and to carry out laboratory work only on the most promising ones. Reviews describe applications in amorphous solid dispersions, lipid-based systems, nanoparticles and long-acting injectables, as well as in the prediction of drug-excipient compatibility.[46] Compared with classical response-surface methods, neural networks and tree-based ensembles can capture non-linear interactions among many variables, but they need more data than a typical small experimental design provides.

Drug delivery systems and nanomedicine

The performance of nanocarriers, such as liposomes, polymeric nanoparticles and micelles, depends on interacting factors including particle size, surface charge, drug loading and release rate. Artificial neural networks and evolutionary algorithms have been used to optimise these attributes and to predict in vitro release and, to a lesser extent, in vivo behaviour.[47] Broader reviews of AI in pharmaceutical technology also describe its use for dosage-form selection, modelling of drug release and the design of targeted and stimulus-responsive systems.[48]

Personalised dosage forms and three-dimensional printing

Three-dimensional (3D) printing can produce tablets whose dose, shape and release profile are tailored to an individual patient, which is attractive for children, older adults and patients who need unusual doses. Not every drug-polymer mixture prints successfully, however. Machine learning models have been trained to predict whether a given formulation will be printable by fused-deposition modelling and how the printed product will perform, replacing a large amount of empirical trial and error.[49] If combined with pharmacogenomic and clinical data, such tools could support on-demand compounding of individualised medicines in hospital pharmacies, although regulation of point-of-care manufacture is still evolving.

Smart manufacturing and quality assurance

Pharmaceutical manufacturing is moving from batch processing towards continuous production and highly instrumented lines,[50],[51] and AI is a key enabling tool. Regulators have encouraged this shift through the Process Analytical Technology (PAT) framework, which promotes timely measurement of critical quality attributes during processing,[52] and through the Quality by Design (QbD) approach described in ICH Q8(R2), which

links product quality to a scientifically established design space.[53] Machine learning models applied to spectroscopic and sensor data can estimate blend uniformity, moisture content or tablet hardness in real time, detect process drift before a batch fails and support predictive maintenance of equipment.[50] "Digital twins", virtual replicas of a process that are continuously updated with plant data, allow operators to test changes in silico before applying them to the real line.[50] Computer-vision systems based on convolutional networks can inspect tablets, capsules and filled vials for defects at speeds beyond manual inspection, and spectral signatures analysed by classifiers can help to flag substandard or falsified products.

Table 2. Applications of AI in pharmaceutical formulation and manufacturing

Area	AI approach	Typical task	Expected benefit	Refs.
Pre-formulation	Regression and tree-based models on physicochemical descriptors	Prediction of solubility, stability and excipient compatibility	Fewer screening experiments	45,46
Dosage-form design	Neural networks, ensemble models	Prediction of disintegration, dissolution and stability from composition	Faster optimisation of recipes	45,46
Nanocarrier design	Neural networks, evolutionary algorithms	Optimisation of particle size, loading and release	More reproducible delivery systems	47,48
3D printing of medicines	Machine learning classifiers and regressors	Printability and quality prediction	Personalised doses and shapes	49
Process monitoring (PAT)	Multivariate and machine learning models on spectra and sensor data	Real-time estimation of quality attributes	Reduced end-product testing	50,52
Continuous manufacturing	Predictive control, digital twins	Deviation detection, process optimisation	Higher yield, lower waste	50,51
Quality control	Convolutional neural networks on images and spectra	Defect inspection, detection of falsified products	Faster, more consistent inspection	50

Applications in Clinical, Hospital and Community Pharmacy

For most pharmacists, the most visible effects of AI will be felt at the point of care. Reviews written for the profession identify several recurring areas: detection and prevention of medication errors and adverse drug events, decision support for prescribing and dosing, adherence support, dispensing automation and inventory management, medication therapy management and patient communication.[9],[10] Table 3 summarises these areas, and the paragraphs below discuss the most developed ones.

Prescription review and prevention of adverse drug events

Adverse drug events are among the most common causes of avoidable harm in health care. Broader evidence reviews conclude that AI is likely to have its greatest impact on patient safety where current strategies are weak and where complex, unstructured data must be combined, a description that fits adverse drug events well.[54] A scoping review of 78 studies identified use cases in both prediction, for example of patient risk or therapeutic response, and early detection, for example of prescribing errors, so that harm can be prevented or limited; it also found that about nine in ten studies reported only technical algorithm performance, and few examined effects in real clinical settings.[55] A systematic review of AI and patient-safety outcomes reached a similar conclusion, noting encouraging results but a need for stronger evidence from routine practice.[56, 57]

Dose individualisation and precision medicine

Many drugs have narrow therapeutic windows and wide differences between patients, for example warfarin, vancomycin, tacrolimus and antiepileptics. Machine learning models that combine clinical variables, laboratory values, concomitant drugs and genotype can estimate the dose most likely to achieve target exposure, and they can integrate multi-omics profiles with clinical records to support precision medicine.[58] For the pharmacist, these tools resemble an extension of pharmacokinetic dosing software: they offer a recommendation and an explanation, and the clinical decision remains with the professional. Prospective trials showing better patient outcomes than standard dosing methods are still scarce for most drugs.

Medication adherence

Non-adherence reduces the benefit of therapy and adds to health-care cost. Technologies for monitoring adherence include smart pill boxes, sensors, mobile applications and video-based confirmation of dose-taking.[59] In a pilot study of patients on anticoagulation, an AI platform that

confirmed ingestion through a smartphone camera and prompted patients improved adherence compared with standard care.[60] Predictive models built on refill history and demographic data can also identify patients at risk of stopping therapy so that pharmacists can intervene early with counselling or reminders.[10]

Dispensing automation, inventory and operations

Robotic dispensing systems and automated compounding devices already operate in many hospitals and high-volume pharmacies, reducing manual picking and selection errors.[10] Forecasting models that learn from past consumption, seasonality and local disease patterns can improve ordering, reduce expiry-related waste and give early warning of shortages.[9] Computer vision can verify the identity of tablets in a dispensing tray or a returned container. These applications are less glamorous than drug discovery, but they free pharmacist time for clinical work.

Patient communication and drug information

Conversational agents and LLMs can answer common questions about how to take a medicine, explain a label in plain language, translate information and draft counselling notes.[17,61] Their usefulness is limited by a property that is especially dangerous in pharmacy: language models can generate fluent, confident statements that are factually wrong, including invented doses, interactions or references, a behaviour known as hallucination.[62] They should therefore be used with human verification, and outputs on dosing or contraindications should be checked against authoritative drug-information sources before reaching the patient.

Community pharmacy services

Community pharmacists are often the most accessible health professionals. AI-supported tools can assist with minor-ailment triage, medication reconciliation, screening for conditions such as diabetes or hypertension, vaccine-eligibility checks and telepharmacy consultations.[10] In settings with a shortage of doctors, including many parts of India, such tools could extend the reach of pharmaceutical care, provided that they are validated locally and that responsibility for decisions is clearly defined.

Table 3. Applications of AI in clinical, hospital and community pharmacy

Function	AI approach	Example use	Current evidence base	Refs.
Order review and error prevention	Machine learning classifiers, anomaly detection	Ranking alerts; flagging atypical orders and interactions	Mostly technical validation; few clinical outcome studies	55,56,57
Dose individualisation	Regression and ensemble models using clinical and genomic data	Dose estimation for narrow-therapeutic-index drugs	Promising; limited prospective trials	58
Adherence support	Computer vision, predictive models, smart devices	Confirming dose-taking; predicting discontinuation	Small pilot studies	59,60
Dispensing and inventory	Robotics, forecasting models, computer vision	Automated picking; demand and shortage forecasting	Established for robotics; emerging for forecasting	9,10
Patient counselling	Chatbots, large language models	Plain-language explanations; drafting notes	Early; accuracy and safety concerns	17,61,62
Community services	Triage and screening algorithms, telepharmacy platforms	Minor-ailment advice; medication reconciliation	Early adoption; local validation needed	10

Pharmacovigilance, Regulatory Affairs, Supply Chain and Pharmacy Education

Pharmacovigilance is the science of detecting, assessing and preventing adverse effects of medicines once they are in use. Its raw material is a large and growing stream of spontaneous reports, electronic health records, literature and, increasingly, social media posts. Statistical disproportionality methods have long been used to detect safety signals in spontaneous-report databases,[63] and machine learning extends these methods by combining more variables, reducing false signals and uncovering patterns that simple two-by-two calculations miss. NLP systems can read free-text narratives and extract drug names, events, dates and outcomes, which is essential because most safety information arrives as unstructured text.[22]

A large part of the workload in a pharmacovigilance department is case processing: receiving reports, coding them in standard terminology, checking for duplicates and assessing seriousness. Industry experience shows that automation based on NLP and machine learning can take over parts of this work, such as case intake and coding, and free trained staff for medical evaluation.[64] A review of the field concluded that AI is already useful for specific tasks, yet it remains essential to validate each tool, to keep humans responsible for causality assessment and to be transparent about the limits of automated output.[65] For pharmacists, who are frequent reporters of adverse reactions, AI-supported reporting interfaces and risk-prediction tools may make reporting faster and the resulting data more complete.

Regulatory science and policy

Regulators are developing frameworks specifically for AI in medicines. In 2023 the US Food and Drug Administration (FDA) published a discussion paper on AI and machine learning in the development of drugs and biological products and invited public comment on issues such as human oversight, data quality and model transparency.[66] In January 2025 it followed with a draft guidance that proposes a seven-step, risk-based framework for establishing the credibility of an AI model for a defined context of use; the guidance applies to AI used to support regulatory decisions on safety, effectiveness or quality, and does not cover AI used in drug discovery or for operational purposes that do not affect patient safety or product quality.[67] The European Medicines Agency (EMA) adopted a reflection paper in 2024 that considers AI across development, authorisation and post-authorisation, and advises developers to engage regulators early when an AI model could affect the benefit-risk balance of a medicine.[68] In January 2026 the two agencies jointly issued ten high-level principles for good AI practice in drug development, stressing human-centred design, a risk-based approach and management of AI systems throughout their life cycle.[69] More broadly, the European Union's Artificial Intelligence Act, which entered into force in 2024, classifies AI systems by risk level and imposes stricter duties on high-risk applications, a category that includes many health-related systems,[70] and the World Health Organization has published ethical principles for AI in health that stress autonomy, safety, transparency, accountability, inclusiveness and sustainability.[71]

Supply chain and hospital logistics

Medicine supply chains are vulnerable to shortages, expiry losses, temperature excursions and counterfeit products. Demand-forecasting models that use sales history, seasonality and epidemiological signals can improve procurement and reduce wastage in hospital and distributor inventories,[9],[10] while sensor data from cold-chain shipments can be analysed to predict spoilage risk. In manufacturing and distribution, image and spectral analysis support the detection of falsified products, as noted earlier.[50] These applications are relatively mature because they use well-structured operational data and carry lower clinical risk than decision support for individual patients.

Pharmacy education

Future pharmacists will need to understand how AI tools work, when to trust them and how to explain them to patients. A scoping review has mapped how AI is being introduced into pharmacy education;[72] the field is young, and evidence on structured curricula and measured learning outcomes remains limited. Opportunities include adaptive learning platforms, AI-simulated patient interviews for counselling practice, automated feedback on case write-ups and support for drug-information searching. The accompanying risks include academic dishonesty, uncritical dependence on tools that can be wrong, and uneven access to technology. Programmes should therefore teach basic AI literacy, critical appraisal of AI output and ethical use, alongside the core clinical sciences.

Opportunities

Faster, cheaper and more productive research and development

By filtering targets and molecules before expensive experiments, AI can shorten early discovery and raise the quality of the candidates that enter the clinic. The early signal of a higher Phase I success rate for AI-discovered molecules, if it holds in larger datasets, would reduce wasted spending on candidates that fail for safety or pharmacokinetic reasons.[44], [33],[34]

Personalised and precision therapy

Combining genomic, clinical, laboratory and lifestyle data allows treatment to be tailored to the individual, with doses and drug choices based on expected response and risk.[58] At the formulation end, 3D printing guided by machine learning could provide dosage forms matched to a patient's needs.[49] Both developments place the pharmacist at the centre of individualisation, because they require expertise in pharmacokinetics, pharmacogenomics and dosage-form science.

Safer medication use

Medication-related harm is largely preventable. AI that predicts which patients are at highest risk, ranks alerts so that the important ones are noticed, and monitors records continuously can help to catch errors earlier.[54],[55] In pharmacovigilance, automated case handling and signal detection can

shorten the time between the first reports of a problem and a regulatory response.[65]

Operational efficiency and workforce capacity
Automation of dispensing, inventory control and documentation can release pharmacist time for activities that need professional judgement and human contact, such as medication reviews, counselling and collaboration with prescribers.[9],[10] Whether time saved is in fact reinvested in patient care depends on how services are organised and paid for, not on the technology alone.

Access and equity
Telepharmacy platforms, symptom-checking tools and multilingual conversational agents may extend pharmaceutical advice to rural and underserved populations. The World Health Organization stresses, however, that AI will widen access only if systems are designed and tested for inclusiveness, since tools trained on data from wealthy populations can perform poorly elsewhere.[71]

An expanding professional role
As AI becomes routine, pharmacists will be asked not only to use tools but also to help select, validate, monitor and explain them, particularly where the tools concern medicines. Clinicians in all fields will need enough understanding of machine learning to recognise its strengths and limits.[73],[74] Pharmacists, with their combined knowledge of drug science, patient care and regulation, are well placed to take on roles in medication-related AI governance, data stewardship and patient education.

Table 4. Principal opportunities created by AI in pharmacy

Domain	Opportunity	Illustrative evidence	Refs.
Research and development	Better candidates, shorter design cycles	Higher early-phase success of AI-discovered molecules; AI-assisted antibiotic and kinase-inhibitor discovery	33,34,35,44
Precision therapy	Individualised doses and dosage forms	Machine learning dosing models; printability prediction for 3D printing	49,58
Medication safety	Earlier detection and prevention of errors and adverse events	Scoping reviews of AI for adverse drug events and patient safety	54,55
Pharmacovigilance	Faster case processing and signal detection	NLP-assisted case handling; review of AI readiness	63,64,65
Operations	Less manual work and less waste	Robotic dispensing; demand forecasting	9,10
Education and profession	New competencies and professional roles	Emerging curricula and AI-literacy needs	72,73,74

Challenges and Limitations
The promise of AI is matched by serious obstacles. They fall into technical, ethical, legal, organisational and professional categories, and they are summarised with possible mitigations in Table 5.

Data quality, availability and bias
AI models learn from data, so their reliability is limited by the data's accuracy, completeness and representativeness. Pharmaceutical and clinical datasets are often small, fragmented, inconsistently coded and affected by missing values, publication bias that favours positive results, and differences in assay methods between laboratories.[20],[30] In health care, models trained on unrepresentative populations can perform worse for under-represented groups. A well-known analysis of a commercial algorithm used to allocate care-management resources showed that, because it used past health-care cost as a proxy for health need, it systematically underestimated the needs of Black patients, and the bias was reduced when the target variable was changed.[75] The lesson for pharmacy is that the choice of outcome variable, the composition of the training data and routine audits for subgroup performance must all be examined before a tool is adopted.

Transparency and interpretability
Many high-performing models, especially deep networks, cannot readily explain why they made a prediction.[25] A pharmacist who cannot see why a system flagged a prescription, or a regulator who cannot see why a model rejected a molecule, has little basis for trust or challenge. Explainability methods help but provide approximations, not complete accounts of model reasoning, and their own reliability needs to be tested. In high-stakes settings simpler, more transparent models may be preferable when their accuracy is similar.

Privacy, security and data governance
AI development often needs large volumes of sensitive health data. Concerns include re-identification of supposedly anonymous records,

secondary use of data without meaningful consent and the concentration of data in a few commercial organisations.[76] In a survey of 501 pharmacy professionals in the Middle East and North Africa, about 59% were concerned about patient data privacy and about 59% about cybersecurity threats.[77] In India, the Digital Personal Data Protection Act, 2023 sets obligations for processing digital personal data, and pharmacies and developers that use patient data in AI systems must comply with it.[78] Technical measures such as de-identification, encryption, access control and training models without centralising data (federated learning) can reduce risk, but they do not replace sound governance.

Accountability, consent and ethics

When an AI-supported decision leads to harm, responsibility may be unclear among the developer, the institution and the professional who relied on the output. Ethical analyses call for patient-centred design, informed consent where AI materially influences care, fairness, and clear lines of accountability.[79],[80] National guidance, such as the Indian Council of Medical Research guidelines on AI in biomedical research and health care, sets out principles that include safety, transparency, accountability and protection of data privacy.[81] As a rule, professionals who use AI recommendations retain responsibility for the care they provide, which is why the "human-in-the-loop" principle is central to current regulatory documents.[68],[69]

Regulatory uncertainty

Regulation is moving, but it is not yet settled. Frameworks differ between regions, several key documents are still drafts or high-level principles, and many pharmacy-practice tools fall in a grey zone between administrative software and medical devices.[66–71] AI models that continue to learn after deployment raise an additional problem, since a change in performance may occur without a formal new approval. Developers and pharmacies should therefore document intended use, monitor performance and engage with regulators where a tool could influence patient safety.

Validation, generalisability and hallucination

Most published AI studies in the medication-safety field report technical performance on retrospective data, and few have tested whether the tool improves outcomes when used in routine care.[55] A model that works in one hospital may fail in another because of differences in patients, prescribing habits and record systems. For LLMs, fabrication of plausible but false statements is a particular concern in a profession where an incorrect dose or interaction can injure a patient.[62] Local validation, prospective evaluation, continuous monitoring and mandatory human verification of high-risk outputs are the main safeguards.[54],[55]

Workforce, training and acceptance

Pharmacy professionals express both enthusiasm and anxiety. In the same regional survey, about 63% were concerned about potential job displacement and about 67% about the absence of legal regulation, and respondents also noted a lack of training in the use of AI tools.[77] Overreliance on automation can erode skills, and "automation bias", the tendency to accept machine output without question, is a recognised hazard.

Cost, infrastructure and the digital divide

Advanced AI tools need reliable data infrastructure, computing capacity, skilled staff and sometimes costly subscriptions. Small community pharmacies and institutions in low- and middle-income settings may be unable to afford them, creating a risk that the benefits of AI accrue mainly to large organisations. Open-source tools, shared national platforms and phased adoption beginning with low-risk operational applications are practical ways to reduce this gap.

Table 5. Key challenges in implementing AI in pharmacy and possible mitigation strategies

Challenge	Why it matters in pharmacy	Possible mitigation	Refs.
Data quality and bias	Models inherit errors and inequities in their data	Representative datasets; subgroup audits; careful choice of outcome variable	20,30,75
Lack of transparency	Professionals cannot verify or challenge predictions	Explainable methods; documentation; preference for simpler models when adequate	25
Privacy and security	Health records are highly sensitive	De-identification, access control, federated learning, legal compliance	76,77,78
Accountability and ethics	Responsibility for AI-assisted harm is unclear	Human-in-the-loop use; consent; ethics review; clear liability rules	79,80,81
Regulatory uncertainty	Rules are evolving and differ by region	Follow risk-based frameworks; early regulator dialogue	66-71
Validation and hallucination	Errors in dose or interaction advice can harm	Prospective trials; local validation; verification against authoritative sources	54,55,62
Workforce	Lack of training and fear of	AI literacy in curricula and continuing	72,77

readiness	displacement	education	
Cost and infrastructure	Uneven access to technology	Open-source tools; shared platforms; phased adoption	77

Future Perspectives

Foundation models and multimodal AI

Foundation models are large networks trained on broad data that can be adapted to many tasks. In medicine they point towards "generalist" systems that combine text, images, laboratory values and omics data in one model, instead of separate narrow tools for each task.[82] For pharmacy, this could mean assistants that read a patient's full record, the product label and the literature together when preparing a medication review. The same flexibility increases the difficulty of validation, because a general system can fail in many unexpected ways.

Self-driving laboratories and digital twins

Closed-loop systems that combine generative design, automated synthesis and testing, and active learning are expected to shorten discovery cycles further.[26],[27] In manufacturing, digital twins and real-time release testing, supported by machine learning, may allow continuous production lines to adjust themselves within a validated design space.[50]

Privacy-preserving collaboration

Federated learning trains a shared model across several institutions without moving patient data out of each site, which could allow hospitals and pharmacy chains to build more representative models while respecting privacy rules.[83]

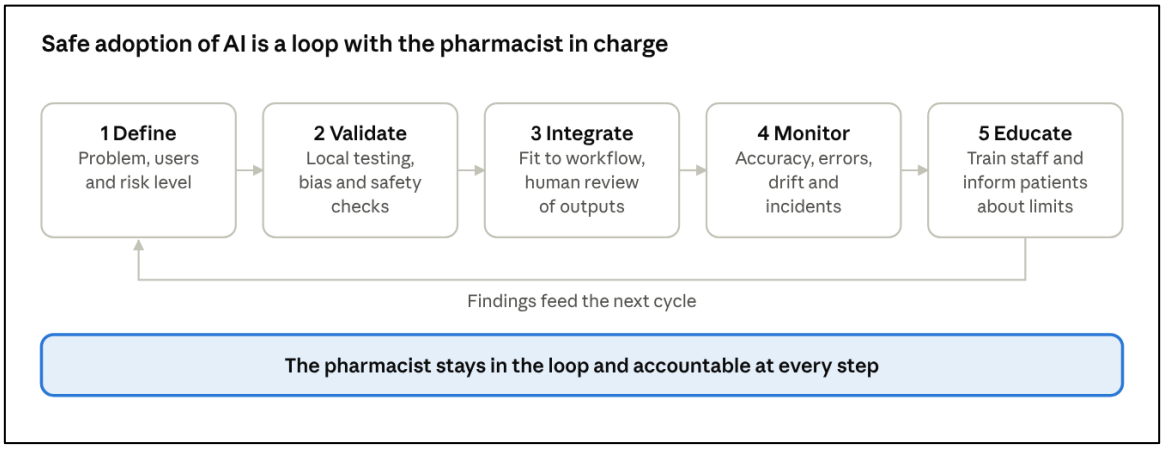


Figure 2. Proposed pharmacist-in-the-loop framework for introducing AI tools into pharmacy practice.

CONCLUSION:

AI is moving from promise to practice across the whole life cycle of medicines. In discovery it helps to find targets, screen and design molecules, predict toxicity, repurpose drugs and plan trials; in pharmaceutics and manufacturing it speeds formulation work and supports real-time quality control; in clinical, hospital and community pharmacy it supports prescription review, dosing, adherence, dispensing and patient communication; and in pharmacovigilance and regulation it improves the handling of safety data and shapes new rules. The opportunities are real: faster and better-targeted development, personalised therapy, safer medicine use and more efficient services. However, the evidence base is uneven. Much of the published work shows technical performance on retrospective data, early clinical results for AI-discovered drugs are encouraging but limited, and persistent problems of data bias, opacity, privacy, accountability, hallucination and unequal access still need to be solved. Regulators are responding with risk-based, lifecycle-oriented frameworks that insist on human oversight. For the pharmacy profession, the most sensible position is neither fear nor uncritical enthusiasm. AI should be treated as a powerful decision-support partner whose outputs are verified by trained professionals who remain accountable for patient care. Pharmacy education, regulation and practice must evolve together so that students and practitioners can use these tools wisely, question them when necessary and ensure that the benefits reach all patients.

CONFLICT OF INTEREST:

The Author declares that there is no conflict of interest.

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