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Artificial Intelligence in Drug Discovery and Development: Applications, Impact, and Challenges

Mariana Costa, Hassan Al-Khaled, Oliver Brown, Sakura Yamamoto, Kwame Mensah

University of São Paulo, Dept. of Pharmacology, Brazil, Qatar University, Dept. of Chemical Engineering - Qatar, University of Melbourne, Dept. of Medicine - Australia, Kyoto University, Dept. of Biotechnology - Japan, University of Ghana, Dept. of Economics - Ghana

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ABSTRACT

Bringing a new medicine to patients remains one of the slowest and most expensive undertakings in applied science, typically requiring more than a decade and billions of dollars, with the great majority of candidates failing along the way. Artificial intelligence (AI) has emerged as a technology with the potential to change this arithmetic, and this review surveys how. We trace the application of machine learning and deep learning across the entire pipeline: target identification from multi-omic data; the prediction of protein structure, whose transformation by AlphaFold has reshaped structure-based design; virtual screening and computer-aided drug design; the generative de novo design of novel molecules; the prediction of absorption, distribution, metabolism, excretion, and toxicity; and applications in clinical development, pharmacology, and drug repurposing. Across these stages the recurring contribution of AI is the same: it compresses the design–make–test–analyse cycle by learning from data to predict which molecules and hypotheses are worth pursuing, allowing scientists to search an astronomically large chemical space with far greater efficiency. We review the accumulating evidence of impact, from AI-guided natural-product and anticancer discovery to therapeutic peptide design and the first AI-originated candidates now entering clinical trials, and we frame the economic logic through which even modest gains in success probability or cycle time translate into large savings. We then examine the challenges that temper the enthusiasm: the dependence on large, high-quality data; the interpretability and generalizability of models; the synthesizability of AI-proposed molecules; regulatory and validation questions; and the organizational and skills barriers to adoption.

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*Corresponding author: mariana.costa@latamdata.br

1. Introduction

Few endeavours in applied medical science are as consequential, or as inefficient, as the discovery and development of new medicines. The process by which a therapeutic hypothesis becomes an approved drug is long, costly, and unforgiving: estimates that capitalize the cost of failures across the pipeline place the average cost of bringing a single new drug to market at roughly 2.6 billion US dollars, spread over a decade or more of work (DiMasi, Grabowski, & Hansen, 2016). The dominant reason is attrition. Most candidates that enter the pipeline never reach patients, failing for lack of efficacy, unacceptable toxicity, or commercial reasons, and because failures are discovered late, after large sums have already been spent, they inflate the cost of the few successes. For decades this arithmetic moved in the wrong direction, with the number of drugs approved per dollar of research spending falling even as the underlying science advanced, a paradox memorably named Eroom's law.

Against this backdrop, artificial intelligence has arrived with unusual promise. The core difficulty of early discovery is one of search: the space of drug-like molecules is estimated to exceed 10^{60} compounds, far too vast to explore by synthesis and assay alone, and the biology that a molecule must engage is correspondingly complex. Artificial intelligence, and in particular machine learning and deep learning, is well suited to precisely this kind of problem, learning patterns from large bodies of chemical and biological data to predict which molecules and which hypotheses are most worth pursuing (Gupta, Srivastava, Sahu, Tiwari, Ambasta, & Kumar, 2021). Over the past decade the technology has moved from the periphery of the field to something close to its centre, touching every stage of the pipeline and, in a growing number of cases, producing candidates that have advanced into human trials (Sarkar et al., 2023).

This review provides an integrated account of that transformation for readers concerned with applied technology in the medical sciences. We pursue four questions. What can AI do at each stage of drug discovery and development? What is the evidence that it delivers real value rather than merely promise? What are the technical and organizational obstacles that keep its impact uneven? And how should a realistic observer weigh its contribution against the hype that inevitably surrounds it? In answering, we draw on the multidisciplinary character of the field, which spans pharmacology, chemistry and chemical engineering, biotechnology, medicine, and the economics of innovation, and we note the growing engagement of clinical and research communities worldwide, including in the Gulf, with AI's role in diagnosis, management, and translational research (Sulthan et al., 2025).

2. Scope and Method

This is a narrative review supported by a structured search of the biomedical and cheminformatics literature. We drew on recent reviews and primary studies indexed in major databases, prioritizing highly cited syntheses and landmark contributions while including current work that reflects the state of the art. The review is organized by the stages of the drug discovery and development pipeline, from target identification through clinical development, so that the reader can see where in the process each class of method contributes. We concentrate on small-molecule discovery, where the literature is deepest and the methods most mature, while noting important extensions to biologics such as therapeutic peptides. The account is interpretive rather than exhaustive, and it is intended to convey the shape of the field and the balance of its promise and its problems rather than to enumerate every study.

3. The AI Toolkit

Before surveying applications it helps to fix the principal methods, because the same families recur across the pipeline. Classical machine learning, including random forests and support-vector machines, remains widely used for predicting molecular properties from engineered descriptors. Deep learning has extended this reach: convolutional and, especially, graph neural networks operate directly on molecular structures represented as graphs, learning features rather than requiring them to be hand-designed. Generative models, variational autoencoders, generative adversarial networks, recurrent networks, and increasingly transformer architectures, do the inverse of prediction, proposing new molecules with desired properties, and reinforcement learning steers that generation toward objectives (Vemula, Jayasurya, Sushmitha, Kumar, & Bhandari, 2023). Natural-language processing, meanwhile, mines the vast textual and sequence literature for target and repurposing hypotheses. Table 2 summarizes these families and their principal uses; the point to carry forward is that a modern discovery campaign typically orchestrates several of them rather than relying on any single technique.

4. Applications Across the Pipeline

Artificial intelligence now contributes at every stage of drug discovery and development, and Figure 1 maps those contributions onto the pipeline. We take the stages in turn.

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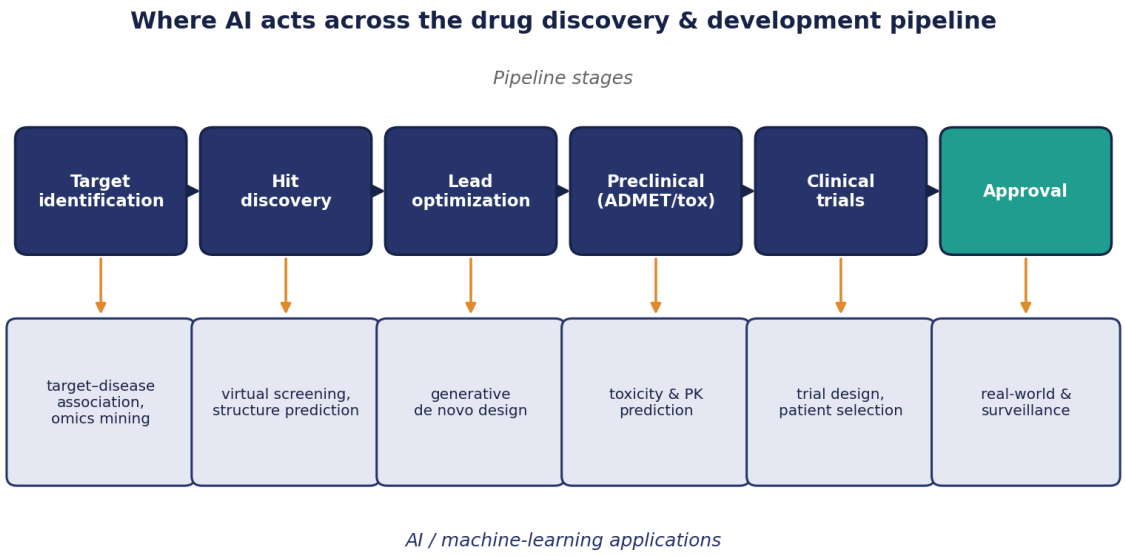

Figure 1. Applications of AI across the drug discovery and development pipeline, from target identification to post-approval surveillance.

4.1 Target identification and validation

Discovery begins with a target, a protein or pathway whose modulation is expected to treat disease, and AI has become a powerful tool for finding and validating targets from the flood of omic data. Machine-learning models integrate genomics, transcriptomics, proteomics, and clinical data to surface associations between biological entities and disease that would be difficult to discern by hand, prioritizing candidate targets for experimental follow-up (Nayarisseri et al., 2021). This multi-omic, AI-driven approach to target discovery is closely allied to precision medicine, and it is an area of active development in neurodevelopmental and other complex diseases where the integration of high-dimensional data is essential (Alshamsi & Alhammadi, 2025).

4.2 Protein structure prediction

Perhaps the single most celebrated advance has come in protein structure prediction. Because a protein's three-dimensional structure governs its function and its druggability, knowing that structure is invaluable for design, yet for most proteins it had never been experimentally solved. The deep-learning system AlphaFold changed this almost overnight, predicting structures from amino-acid sequence with an accuracy that approaches experiment for many proteins (Jumper et al., 2021). The consequences for drug discovery are substantial, opening previously inaccessible targets to structure-based design, though careful appraisals note that predicted static structures do not capture the conformational dynamics and binding-induced changes that rational design ultimately requires (Schauperl & Denny, 2022). Structure prediction has, in short, removed one long-standing bottleneck while sharpening attention on the ones that remain.

4.3 Virtual screening and computer-aided design

With a target and, increasingly, its structure in hand, the next task is to find molecules that engage it. AI has transformed virtual screening, in which computational models triage vast compound libraries to identify likely binders before any synthesis, and machine-learning scoring functions now routinely outperform older physics-based approaches on many tasks (Parvatikar et al., 2023). Integrated into the broader practice of computer-aided drug design, these methods let a campaign screen billions of molecules in silico, concentrating scarce experimental effort on the most promising candidates and so compressing the earliest and most combinatorially explosive phase of discovery.

4.4 Generative design and lead optimization

The most striking capability AI brings is generative: rather than only selecting from existing libraries, models can propose entirely new molecules designed to satisfy multiple objectives at once. Early work showed that sequence-based generative models tuned by reinforcement learning could design molecules predicted, and in some cases experimentally confirmed, to be active against a chosen target (Olivecrona, Blaschke, Engkvist, & Chen, 2017). The field has since matured into a rich toolkit of generative architectures and optimization strategies, some of them validated experimentally in academic and industrial settings (Du et al., 2024), and

systematic reviews now catalogue the model families and the challenges that remain (Martinelli, 2022). This generative capacity is what most distinguishes AI-driven discovery from its predecessors: it turns design from a search among known molecules into the creation of new ones.

4.5 ADMET and toxicity prediction

Because so much attrition stems from poor pharmacokinetics or unexpected toxicity discovered late, predicting these properties early is among AI's most economically valuable contributions. Machine-learning models estimate absorption, distribution, metabolism, excretion, and toxicity from molecular structure, letting teams filter out liabilities before committing to synthesis and animal testing (Vemula et al., 2023). Moving these predictions earlier in the pipeline directly attacks the late-failure problem that inflates the cost of the whole enterprise.

4.6 Clinical development, pharmacology, and repurposing

AI's reach extends beyond the laboratory into clinical development and pharmacology. Machine learning supports clinical-trial design and patient stratification, models pharmacokinetics and dosing, and helps interpret the complex data that clinical pharmacology generates (Ryan, Maclean, Balston, Scourfield, Shah, & Ross, 2024). Drug repurposing, identifying new uses for existing, already-safe drugs, is a particularly attractive application because it short-circuits much of the early pipeline, and AI's ability to mine relationships across drugs, targets, and diseases makes it well suited to the task. Table 1 maps the principal applications onto the pipeline stages.

4.7 Toward autonomous discovery: language models and self-driving laboratories

A frontier now taking shape promises to knit these individual applications into something more integrated. Large language models, having demonstrated fluency with the textual and symbolic representations of chemistry and biology, are beginning to serve as reasoning layers that can plan experiments, retrieve and synthesize the literature, and coordinate specialized predictive tools, moving the field toward assistants that participate in discovery rather than merely score molecules. Coupled with laboratory automation, this points toward the self-driving laboratory, a closed loop in which AI proposes candidates, robotic systems synthesize and test them, and the results feed directly back into the models, compressing the design–make–test–analyse cycle from months to days (Huanbutta et al., 2024).

These developments are genuinely promising, but they also concentrate the field's existing challenges rather than dissolving them. An autonomous loop is only as trustworthy as the data and models that drive it, and the interpretability and validation questions examined below become more, not less, pressing when a human is further from each decision. The realistic near-term picture is therefore one of increasingly capable assistance and partial automation rather than fully autonomous discovery, with the human scientist remaining central to judgement, hypothesis, and the interpretation of biological meaning. The frontier is moving quickly, and it is precisely where the balance between promise and prudence most needs to be held.

Table 1. AI applications mapped to the drug discovery and development pipeline.

Pipeline stage	AI application	Illustrative evidence
Target identification	Multi-omic mining; target–disease association.	Nayarisseri et al. (2021); Alshamsi & Alhammadi (2025)
Structure prediction	Sequence-to-structure prediction (AlphaFold).	Jumper et al. (2021); Schauperl & Denny (2022)
Hit discovery	Virtual screening; ML scoring functions.	Parvatikar et al. (2023)
Lead optimization	Generative de novo design; multi-objective optimization.	Olivecrona et al. (2017); Du et al. (2024)
Preclinical	ADMET and toxicity prediction.	Vemula et al. (2023)
Clinical & beyond	Trial design, pharmacology, repurposing, surveillance.	Ryan et al. (2024); Huanbutta et al. (2024)

Table 2. Principal AI method families used in drug discovery.

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Method family	Typical use	Notes
Classical ML (RF, SVM)	Property prediction from descriptors.	Robust, interpretable, data-efficient.
Deep learning (CNN, GNN)	Learning features from molecular graphs/images.	Strong with large data.
Generative models (VAE, GAN, RNN, transformer)	De novo molecule generation.	Enables design, not just selection.
Reinforcement learning	Steering generation toward objectives.	Multi-objective optimization.
NLP / large language models	Literature mining; target & repurposing hypotheses.	Emerging, fast-moving.

5. Impact and Evidence

The value AI creates in discovery can be understood through a simple economic lens that also clarifies where its leverage lies. The risk-adjusted cost of producing one approved drug depends on the cost incurred at each stage and on the probability of surviving it. If C_i is the cost of stage i and p_i the probability of a candidate passing it, the expected cost per launched drug is, schematically,

$$E[C] = \left(\sum_i C_i\right) / \left(\prod_i p_i\right),$$

where the product of the per-stage success probabilities, the cumulative probability of a candidate surviving the whole pipeline, sits in the denominator. This expression makes AI's two avenues of impact explicit. By improving decisions, screening out likely failures early and proposing better candidates, AI raises the p_i, especially at the stages where attrition is most costly; and by accelerating the design–make–test–analyse cycle it lowers the effective C_i for a given amount of exploration. Because the success probabilities multiply, even modest improvements at several stages compound into a large reduction in the cost per approved drug, which is why the economic case for AI does not rest on any single dramatic breakthrough. Figure 2 depicts the closed loop that AI accelerates.

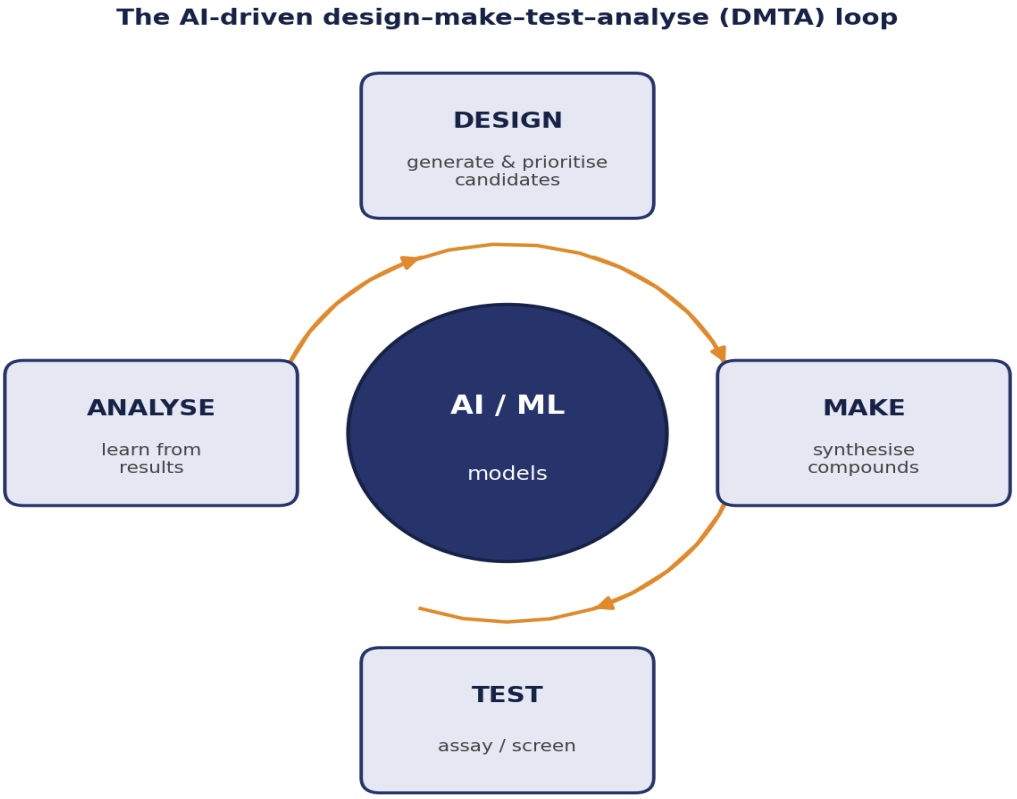

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Figure 2. The AI-driven design–make–test–analyse (DMTA) loop, which machine-learning models accelerate at each turn.

Concrete evidence of impact has accumulated across therapeutic areas. In natural-product discovery, a field long constrained by the labour of isolating and characterizing compounds, AI is accelerating the identification of promising molecules and the elucidation of their structures (Mullowney et al., 2023; Gangwal & Lavecchia, 2025). In oncology, AI is being applied across the discovery and development of anticancer agents, from target identification to the prediction of response (Sarvepalli & Vadarevu, 2025). The generative design of therapeutic peptides has advanced toward increasingly autonomous pipelines (Goles et al., 2024), and AI is now embedded across the pharmaceutical industry's activities from discovery through formulation, manufacturing, quality control, and post-market surveillance (Huanbutta et al., 2024). Most tellingly, molecules originated or optimized with AI have begun to enter clinical trials, moving the field from in-principle demonstration toward clinical reality, even if the ultimate test, AI-originated drugs reaching approval, still lies ahead.

6. Challenges and Limitations of the Technology

The enthusiasm the field generates should be tempered by a clear view of its obstacles, which are substantial and largely shared across applications. The most fundamental is data: AI models are only as good as the data that train them, and high-quality, well-annotated, and unbiased chemical and biological data remain scarce, expensive, and often proprietary, while negative results, which are highly informative, are systematically under-reported (Gupta et al., 2021). A second challenge is interpretability: many high-performing models are opaque, and a prediction that a molecule will be active or toxic is less useful to a medicinal chemist, and less acceptable to a regulator, if the reasoning behind it cannot be inspected. A third is generalizability: models often perform well on data resembling their training set but degrade on genuinely novel chemistry, precisely where discovery most needs them.

Further obstacles are as much practical as they are algorithmic. Generative models can propose molecules that are potent on paper but difficult or impossible to synthesize, so that synthesizability must be built into the objective rather than assumed. Regulation and validation are still maturing, and the path by which an AI-derived claim is accepted in a submission is not yet fully settled, which counsels caution in high-stakes applications. And, as with any advanced technology, skills and integration are limiting: realizing value requires teams that span data science, chemistry, biology, and clinical insight, and organizations that can embed AI into their workflows rather than bolting it on. Table 3 summarizes these challenges and the directions in which the field is responding.

Table 3. Challenges to AI in drug discovery and emerging responses.

Challenge	Why it matters	Emerging response
Data quality & availability	Models inherit gaps and biases; negatives under-reported.	Data sharing, curation, standards; active learning.
Interpretability	Opaque predictions resist scientific and regulatory scrutiny.	Explainable AI; physically grounded models.
Generalizability	Models degrade on novel chemistry.	Robust validation; uncertainty quantification.
Synthesizability	Proposed molecules may be unmakeable.	Synthesis-aware generation; retrosynthesis models.
Regulation & validation	Acceptance pathways still maturing.	Prospective validation; regulatory engagement.
Skills & integration	Value needs cross-disciplinary teams.	Training; integrated platforms and workflows.

7. Discussion

Read as a whole, the evidence supports a measured but genuinely optimistic conclusion. Artificial intelligence has moved from a promising adjunct to an established and increasingly indispensable component of drug discovery, contributing across the pipeline and, in a growing number of cases, producing candidates that reach the clinic. The transformation of protein structure prediction and the maturation of generative design are

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advances of real substance, not merely of marketing, and the economic logic set out above explains why the aggregate effect of many incremental improvements can be large. At the same time, the field has not, and should not claim to have, abolished the fundamental difficulty of making medicines: biology remains complex, data remain imperfect, and the clinic remains the ultimate and unforgiving arbiter. The honest summary is that AI has shifted the odds and the pace of early discovery meaningfully, without yet transforming the end-to-end success rate, which will be known only as more AI-originated candidates complete clinical development.

Three implications follow. First, because the binding constraints are now data, validation, and integration rather than algorithmic capability, the highest-value investments are increasingly in shared, high-quality data and in rigorous prospective validation rather than in ever-more-elaborate models. Second, the multidisciplinary nature of the enterprise means that its progress depends on collaboration across chemistry, biology, medicine, engineering, and the economics of innovation, no single discipline commands the whole. Third, the diffusion of these methods beyond a handful of leading firms and countries is where much of the future social value lies, and the growing engagement of clinical and research communities across regions, including studies of AI's role in diagnosis and translational research in the Gulf, signals that the technology's reach is broadening (Sulthan et al., 2025; Alshamsi & Alhammadi, 2025). The task ahead is less to prove that AI can contribute, which is now clear, than to build the data, validation, and collaboration through which its contribution can be made reliable, general, and widely shared.

A note of proportion is warranted here, because the field is as prone to hype as any in contemporary science. It is one thing to accelerate the earliest phases of discovery, where AI's evidence is strongest, and another to move the end-to-end probability that a program yields an approved medicine, which is determined overwhelmingly in the clinic by human biology that no model yet captures fully. The candidates AI has helped bring into trials are an important milestone, but a milestone is not a destination, and the decisive evidence, whether AI-originated drugs succeed in late-stage trials at rates better than the historical norm, will accumulate only over years. Holding this distinction clearly in view protects the field from both premature triumphalism and reflexive scepticism, and it directs attention to the measurement that matters: not how many molecules a model can generate, but how many patients are eventually helped.

Table 4. Priority actions for realising the value of AI in drug discovery, by stakeholder.

Stakeholder	Near-term action	Longer-term action
Research organisations	Invest in data curation and FAIR data practices; pilot AI in defined use cases.	Embed AI in integrated DMTA workflows; build self-driving-lab capability.
Regulators	Clarify expectations for validating AI-derived evidence.	Develop standards for explainability and prospective validation.
Funders & industry	Support shared, high-quality benchmark datasets.	Fund open pre-competitive data and negative-result reporting.
Universities	Train cross-disciplinary talent spanning data, chemistry, and biology.	Sustain talent pipelines and academia–industry collaboration.
Global & regional bodies	Broaden access to tools and data beyond leading hubs.	Enable equitable participation and capacity-building worldwide.

8. Limitations

This review has limitations. As a narrative synthesis it represents the principal themes and influential works rather than an exhaustive census, and its selection reflects judgement. It is weighted toward small-molecule discovery, so its conclusions transfer less securely to biologics, cell and gene therapies, and vaccines, where AI's role is developing along partly different lines. Much of the impact evidence, particularly claims of accelerated timelines, comes from industry reports and case studies whose generalizability is uncertain, and the economic expression we present is illustrative rather than a validated model. The field is also moving exceptionally quickly, especially at the frontier of large language models and autonomous experimentation, so some conclusions are necessarily provisional and will require revision as clinical outcomes of AI-derived candidates mature.

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9. Conclusion

Artificial intelligence has become one of the defining technologies of contemporary drug discovery and development, contributing at every stage from target identification and protein structure prediction through generative molecular design, property prediction, and clinical development. Its core contribution is consistent across these applications: by learning from data to predict which molecules and hypotheses merit pursuit, it lets scientists explore an otherwise intractable space more efficiently, compressing the design–make–test–analyse cycle and attacking the late-failure problem that makes drug development so costly. The evidence of real impact is now substantial, extending to candidates in clinical trials, even as significant challenges in data, interpretability, generalizability, synthesizability, regulation, and skills remain. The realistic assessment is therefore neither dismissal nor uncritical enthusiasm but recognition that AI has permanently changed how medicines are discovered, and that realizing its full promise will depend less on further algorithmic ingenuity than on the quality of data, the rigour of validation, and the breadth of collaboration with which it is applied.

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