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Artificial intelligence in drug development: Transforming the journey from molecule to medicine

B. Dhanvandhini[1], M. Jayanthi[2], S. P. Preetha[3] and R. Yogeswari[4]

[1]PhD Scholar, Department of Veterinary Pharmacology and Toxicology, Madras Veterinary College, Chennai
[2]Assistant Professor, Department of Veterinary Pharmacology and Toxicology, Veterinary College and Research Institute, Theni
[3]Professor, Department of Veterinary Pharmacology and Toxicology, Madras Veterinary College, Chennai
[4]Associate Professor, Department of Veterinary Pharmacology and Toxicology, Madras Veterinary College, Chennai

**Corresponding Author: dhanu2301vet@gmail.com*

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INTRODUCTION

Developing a new drug is a long, expensive and uncertain process. From identifying a promising biological target to obtaining regulatory approval, a drug may take many years and require extensive laboratory and clinical testing. Thousands of compounds may be investigated, yet only a small proportion eventually become medicines.

Artificial intelligence (AI) is emerging as a powerful technology capable of changing this traditional drug-development process. Machine learning, deep learning, generative AI and other computational approaches can analyse enormous quantities of chemical, biological and clinical data and identify patterns that may be difficult to detect using conventional approaches.

AI is therefore increasingly being used not to replace scientists, but to help them make better decisions about **which targets to study, which molecules to synthesize and which candidates should proceed to further testing**.

AI IN TARGET IDENTIFICATION

The first step in many drug-discovery programs is identifying an appropriate biological target. Diseases can involve complex interactions between genes, proteins, signalling pathways and cellular processes. Finding the most relevant target from this enormous biological network is challenging. AI can integrate genomic, transcriptomic, proteomic and clinical information to identify relationships between diseases and potential therapeutic targets. Machine-learning models can analyse large biological datasets and identify genes or proteins associated with disease progression.

AI can also contribute to **drug repurposing**. Instead of developing a new drug from the beginning, computational models can identify existing medicines that may have therapeutic effects against another disease. This approach can potentially reduce development time because some safety and pharmacological information may already be available.

VIRTUAL SCREENING: SEARCHING MILLIONS OF MOLECULES

One of the important applications of AI is virtual screening. Traditional drug discovery may require researchers to experimentally test large chemical libraries. This can be expensive and time-consuming. AI can act as an initial filter by predicting which molecules are most likely to interact with a particular target. The process can be visualized as:

Large chemical library → AI prediction → Virtual screening/docking → Selected compounds → Experimental validation

AI can therefore reduce the number of molecules that need to be synthesized and tested experimentally. However, a computational prediction is not equivalent to biological activity. A molecule predicted to bind strongly to a protein may fail in cellular, animal or clinical studies. Experimental validation therefore remains essential.

AI FOR DESIGNING NEW DRUG MOLECULES

Perhaps the most exciting development is the use of **generative AI for drug design**.

Conventional medicinal chemistry often modifies existing compounds to improve their properties. Generative AI can instead propose new molecular structures based on desired characteristics.

For example, researchers may want a molecule with:

- High affinity for a specific target
- Good solubility
- Suitable molecular weight

- Good oral absorption
- Metabolic stability
- Low toxicity
- High selectivity

AI models can generate and rank molecules according to multiple properties simultaneously. This concept, known as **multi-parameter optimization**, is particularly important because a successful drug must satisfy several requirements at the same time. A molecule with excellent target binding but poor absorption or severe toxicity is unlikely to become a successful drug.

AI IN PHARMACOKINETICS AND ADME

A drug must reach its target in sufficient concentration to produce its therapeutic effect. Therefore, understanding **ADME—absorption, distribution, metabolism and excretion—is essential**. AI models can predict several pharmacokinetic properties during the early stages of drug development. These include oral absorption, plasma protein binding, metabolic stability, blood–brain barrier penetration, cytochrome P450 interactions and drug clearance.

Early prediction of poor ADME properties can help researchers remove unsuitable compounds before investing significant resources in further development. This represents an important advantage of AI: **failure can potentially be identified earlier and at lower cost**.

AI IN TOXICOLOGY

Safety is one of the biggest challenges in drug development. A compound may demonstrate excellent pharmacological activity but ultimately fail because of toxicity. AI-based toxicology models can analyse existing chemical and toxicological datasets to predict possible adverse effects, including:

- Hepatotoxicity
- Cardiotoxicity
- Nephrotoxicity
- Genotoxicity
- Mutagenicity
- Drug-induced organ injury

Such approaches may also contribute to the **3Rs principle—Replacement, Reduction and Refinement**—by helping identify unsuitable compounds before extensive animal experimentation. Nevertheless, computational toxicology cannot completely replace experimental safety assessment. Toxicity may depend on metabolism, dose, exposure duration, species and interactions between multiple biological systems.

AI IN CLINICAL TRIALS

AI is also moving beyond laboratory drug discovery into clinical development. Clinical trials require appropriate patient selection, recruitment, monitoring and analysis. AI can analyse clinical and biological information to identify patients who are more likely to respond to a particular treatment. This is particularly relevant to **precision medicine**, where treatment decisions are increasingly based on the molecular and genetic characteristics of individual patients. AI may also assist with clinical-trial recruitment, identification of suitable trial sites, analysis of clinical data and detection of potential safety signals. However, compared with early drug discovery, the application of AI in clinical development remains less mature, and evidence demonstrating consistent improvement in clinical outcomes is still emerging.

GENERATIVE AI: THE NEXT STEP

The emergence of generative AI and large language models has expanded the possibilities further.

AI systems can now assist researchers with:

- Scientific literature analysis
- Biological hypothesis generation
- Drug–target relationship identification
- Chemical structure analysis
- Experimental planning
- Data interpretation
- Scientific knowledge organization

The future may involve AI systems capable of connecting different stages of drug development.

For example:

Disease → Target → Molecule design → Virtual screening → ADME prediction → Toxicity prediction → Experimental validation

The experimental results can then be fed back into the AI system, creating a continuous **design–make–test–learn** cycle.

CHALLENGES AND LIMITATIONS

Despite its promise, AI is not a magic solution to the problems of drug development. The first challenge is **data quality**. AI models depend heavily on the quality and diversity of their training data. Poor-quality or biased datasets can produce unreliable predictions.

A second issue is **interpretability**. Some sophisticated AI models can produce accurate predictions without clearly explaining how they reached those conclusions.

Third, computational predictions require **experimental validation**. A molecule that looks promising on a computer may fail in a biological system.

Finally, regulatory agencies must determine how AI-generated evidence should be evaluated. The U.S. FDA has already proposed a risk-based framework for assessing the credibility of AI models used to support regulatory decisions involving drugs and biological products.

Thus, the future is unlikely to be **AI versus scientists**. Instead, it will be **AI + scientists + laboratory experimentation**.

FUTURE PERSPECTIVE

The ultimate goal of AI in drug development should not be to generate the largest number of molecules or the most sophisticated algorithms. The real measure of success is whether AI can help produce **safer, more effective medicines in a faster and more reliable way**. AI has the potential to reduce unnecessary screening, improve candidate selection and identify promising therapeutic strategies that might otherwise remain undiscovered.

However, the transition from a computer-generated prediction to an approved medicine still requires medicinal chemistry, pharmacology, toxicology, preclinical research, clinical trials and regulatory evaluation. The future of drug development will therefore be a partnership between computational intelligence and experimental science.

CONCLUSION

Artificial intelligence is transforming drug development from a predominantly trial-and-error process into an increasingly data-driven and predictive discipline. Its applications now extend from target identification and virtual screening to molecular design, pharmacokinetic prediction, toxicology and clinical development.

The technology is powerful, but its greatest value lies not in replacing researchers. Instead, AI can help scientists **ask better questions, prioritize experiments and make better-informed decisions**.

The real revolution will occur when AI predictions and laboratory experimentation become part of a continuous, integrated drug-development process—bringing promising discoveries from **molecule to medicine** more efficiently and safely.

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