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Editorial

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Reimagining Drug Delivery: Can Artificial Intelligence Transform the Pharmaceutical Research?

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Looking back at history, many scientists working on the development of drug delivery systems mainly relied on their scientific knowledge, experience, and judgment rather than advanced technologies. Mostly, the formulation can be developed by selecting suitable polymers, controlling particle size, screening appropriate excipients, and performing laboratory experiments until the desired formulation shows satisfactory performance. A researcher has various choices while developing a formulation, such as the number of polymers, the excipient, the concentration, the temperatures, the mixing speed and so on. Because there are various possible combinations, testing them all in the laboratory is not possible, making drug formulation development time-consuming and expensive. The conventional approach has yielded extended-release tablets, liposomes, and lipid nanoparticles that have delivered mRNA vaccines to a waiting world. Yet it remains slow, expensive and persistently experimental. The formulation design space comprises an enormous number of possible combinations of materials, composition, and process parameters, making exhaustive evaluation using conventional approaches, such as one-factor-at-a-time studies and design of experiments (DoE), impractical [1,2]. Against a backdrop where the development of new medicines now costs more than US$2.5 billion and needs more than a decade to develop, and very few (2%) drug candidates enter the market [3], the challenge is not only to ensure the molecule works effectively, but also that it reaches its intended target site efficiently.

Artificial intelligence (AI) and machine learning (ML) offer a new approach to drug formulation development. These approaches learn the complex relationships between formulation parameters and their performance via analysing the experimental data. They can predict the behaviour of novel systems that have not yet been developed [1]. Initially developed for target identification and lead optimisation, AI and ML have evolved into powerful computational tools used in drug discovery, formulation, and manufacturing processes [4,5]. As the global drug-delivery market is expected to reach US$2.5 trillion by 2029 [2], nowadays there is an increasing need to replace extensive experimental studies with data-driven approaches.

Recent developments have proven the significant potential of AI and ML in pharmaceutical formulation. Models such as support vector regression, random forests, gradient boosting, and neural networks can predict important quality attributes of nanocarriers, such as average particle size, polydispersity index, and drug encapsulation efficiency, based on formulation composition [5,6]. Combined with Bayesian optimisation and active learning, these models can improve the efficiency and continuous development of pharmaceutical formulations by guiding the selection of subsequent experiments [1]. Additionally, an AI-driven approach is being employed for the rational design of nanocarriers, stimuli-responsive drug delivery systems, and closed-loop systems that release their payload in response to physiological triggers [6,7], as well as for the personalised and theranostic delivery required for precision medicines [8,9]. AI does not replace formulation scientists; rather, it enhances decision-making by providing data-driven predictions and recommendations, while final decisions remain with researchers.

Although they have significant potential, various challenges remain, with data availability and quality posing major limitations. The predictive performance of ML models fundamentally depends on the robustness of the underlying dataset. In pharmaceutical formulation research, existing data are frequently limited, proprietary, heterogeneous, and biased regarding effective formulations. Without deliberate standardisation and validation, models can overfit and generalise poorly, leading to inaccurate predictions outside the training data's domain [5]. Recent studies have proposed a “Rule of Five” framework for the development of trustworthy formulation models, emphasising a data set containing

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500 samples, covering at least 10 drugs and major excipients, appropriate molecular descriptors, the inclusion of critical process parameters, and demonstrable model interpretability [2]. Implementing these principles is necessary to ensure the robustness and generalisability of AI-driven pharmaceutical formulations.

Another major challenge is model interpretability. Regulatory authorities and patients require a clear understanding of why a formulation is expected to exhibit specific features. Therefore, black-box models with limited interpretability remain difficult to reconcile with the mechanistic principles that underpin pharmaceutical sciences [3,6]. Furthermore, computational predictions should be considered hypotheses rather than definitive outcomes, as in silico study results cannot replace rigorous experimental and clinical validation to establish the safety, stability, and therapeutic efficacy of drug delivery systems. Consequently, AI and ML should be viewed as complementary tools that improve, rather than replace, scientific expertise and evidence-based decision making [10].

Promisingly, the regulatory frameworks are evolving in parallel with technological advances. Regulatory agencies such as the US Food and Drug Administration (FDA) have increasingly recognised and actively supported the role of AI across the drug development while emphasising requirements related to data quality, model transparency, and lifecycle oversight [2]. The successful integration of AI into the pharmaceutical industry requires strict adherence to the principles of reproducibility, transparency, and scientific evidence. Computational approaches that fail to meet these standards cannot be regarded as genuine innovations.

In the development of AI-driven pharmaceutical research, three priorities are crucial: first, open and standardise formulation datasets, including negative results, to expand model reliability. Second, interpretable and physics-informed models should integrate ML with principles of transport, thermodynamics and materials sciences [1,6]. Third, stronger, closer collaboration between data scientists and formulation experts is essential to ensure that algorithm development remains aligned with pharmaceutical challenges [3].

AI alone cannot reimagine drug delivery or replace the scientific foundations of pharmaceutical research. However, when integrated with robust pharmaceutical principles, high-quality data, and rigorous validation, it can accelerate and advance the development of safe and effective drug delivery systems. AI is expected to reshape the approach of drug delivery, making tangible the way for more precise, patient-centred, and effective therapeutic solutions.

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References

1. Ros H, Chan N, Cook MT, Shorthouse D. Artificial intelligence and machine learning guided optimization in drug delivery. Adv Drug Deliv Rev. 2026;232:115781. https://doi.org/10.1016/j.addr.2026.115781

2. Wu Y, Wang N, Xiong P, Wang R, Deng J, Ouyang D. Artificial intelligence for drug delivery: yesterday, today and tomorrow. Acta Pharm Sin B. 2026;16(4):2068–2092. https://doi.org/10.1016/j.apsb.2025.09.022

3. Kant S, Deepika, Roy S. Artificial intelligence in drug discovery and development: transforming challenges into opportunities. Discov Pharm Sci. 2025;1:7. https://doi.org/10.1007/s44395-025-00007-3

4. Gholap AD, Uddin MJ, Faiyazuddin M, Omri A, Gowri S, Khalid M. Advances in artificial intelligence for drug delivery and development: a comprehensive review. Comput Biol Med. 2024;178:108702. https://doi.org/10.1016/j.compbiomed.2024.108702

5. Serrano DR, Luciano FC, Anaya BJ, Ongoren B, Kara A, Molina G, et al. Artificial intelligence (AI) applications in drug discovery and drug delivery: revolutionizing personalized medicine. Pharmaceutics. 2024;16(10):1328. https://doi.org/10.3390/pharmaceutics16101328

6. Singh S, De A. The paradigm shift in therapeutics: a comprehensive review of artificial intelligence in drug delivery systems. RSC Pharm. 2026;3:645–653. https://doi.org/10.1039/d5pm00235d

7. Jena GK, Patra CN, Jammula S, Rana R, Chand S. Artificial intelligence and machine learning implemented drug delivery systems: a paradigm shift in the pharmaceutical industry. J Bio-X Res. 2024;7:0016. https://doi.org/10.34133/jbioxresearch.0016

8. Vora LK, Gholap AD, Jetha K, Thakur RRS, Solanki HK, Chavda VP. Artificial intelligence in pharmaceutical technology and drug delivery design. Pharmaceutics. 2023;15(7):1916. https://doi.org/10.3390/pharmaceutics15071916

9. Panchpuri M, Painuli R, Kumar C. Artificial intelligence in smart drug delivery systems: a step toward personalized medicine. RSC Pharm. 2025;2:882–914. https://doi.org/10.1039/d5pm00089k

10. Gormley AJ. Machine learning in drug delivery. J Control Release. 2024;373:23–30. https://doi.org/10.1016/j.jconrel.2024.06.045

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