Journal of Pharmaceutical Research and Integrated Medical Sciences (JPRIMS)
ISSN: 3049-1681 | Vol. 03, Issue-03, March-2026 | pp.-17-31

ORIGINALARTICLE https://aktpublication.com/index.php/jprims/index

Artificial Intelligence in Pharmacology and Pharmaceutics: From Drug Discovery to Clinical Translation

Amrut Arun Swami[1], S. Shruti[2], Perbhat Kansal[1], Gayathridevi S[3], Anand Bhide[1*]
[1]Dr. S. S. Tantia Medical College, Hospital and Research Centre, Sri Ganganagar, Rajasthan.
[2]Sri Ganganagar College of Ayurvedic Science and Hospital, Sri Ganganagar, Rajasthan. Email:
[3]Senior scientific officer, Chemistry section, Regional Forensic Science Laboratory
[4]MIMER Medical College, Talegaon, Pune, Maharashtra.
***Corresponding Email: dranandrbhide@gmail.com**

Abstract:

Artificial intelligence (AI) has emerged as a transformative tool in pharmacology and pharmaceutics, enabling accelerated drug discovery, formulation optimization, and clinical translation. Machine learning, deep learning, and predictive modeling improve target identification, lead optimization, and personalized therapy. AI-driven platforms facilitate high-throughput screening, pharmacokinetic/pharmacodynamic (PK/PD) modeling, and nanocarrier design, reducing time, cost, and attrition rates. This review highlights the applications of AI across the drug development pipeline, from molecular discovery to regulatory submission, and discusses challenges, ethical considerations, and future perspectives in precision pharmacotherapy.

Keywords: Artificial Intelligence, Pharmacology, Pharmaceutics, Drug Discovery, PK/PD Modeling, Nanomedicine, Clinical Translation.

Received: Dec. 28, 2025 **Revised: Jan. 22, 2026** **Accepted: Feb. 26, 2026** **Published: March. 19, 2026**

DOI: https://doi.org/10.64063/3049-1681.vol.3.issue3.2

https://aktpublication.com/index.php/jprims/issue/archive

1. Introduction

The conventional process of drug development is an inherently complex and lengthy endeavor, often taking over a decade to bring a single therapeutic molecule from the discovery phase to clinical approval [1]. This process is not only time-consuming but also extremely costly, with billions of dollars invested and attrition rates exceeding 90% at various stages of the pipeline. Many promising drug candidates fail to progress beyond preclinical or early clinical stages due to issues related to efficacy, safety, pharmacokinetics, or manufacturability [2]. This high failure rate poses a substantial challenge to both the pharmaceutical industry and healthcare systems

worldwide, delaying the delivery of effective therapies to patients and increasing the overall economic burden [3].In recent years, Artificial Intelligence (AI) has emerged as a powerful tool to address these long-standing challenges in drug discovery and development [4]. By harnessing massive datasets, advanced computational algorithms, and predictive modeling techniques, AI introduces a paradigm shift from traditional trial-and-error approaches to data-driven and knowledge-based decision-making. Unlike conventional methods, which are often linear and resource-heavy, AI enables faster, more accurate, and more cost-effective predictions at every stage of drug development [5].

One of the most impactful applications of AI lies in drug discovery, where machine learning and deep learning algorithms are used to identify novel therapeutic targets, design and optimize lead compounds, repurpose existing drugs, and predict ligand–receptor interactions with high precision [6]. In formulation development**,** AI contributes significantly to optimizing critical parameters such as solubility, stability, dissolution, bioavailability, and controlled-release properties, which are essential for ensuring therapeutic efficacy and patient compliance [7]. Moreover**,** AI-driven clinical translation plays a crucial role in predicting pharmacokinetic and pharmacodynamic profiles, anticipating adverse drug reactions, and tailoring drug therapies to individual patient characteristics—ushering in the era of personalized medicine.

Beyond accelerating timelines and reducing costs, AI also enhances the predictive accuracy of drug development strategies, helping researchers identify potential risks earlier in the pipeline [8]. This allows for smarter allocation of resources, fewer clinical trial failures, and improved regulatory outcomes. As a result, AI is not merely an add-on technology but a disruptive force reshaping the entire pharmaceutical landscape**,** bridging the gap between bench research and bedside application [9].

2. AI in Drug Discovery and Target Identification

The early stages of drug discovery are often the most critical, as they lay the foundation for the entire development pipeline. Traditionally, this process relies on extensive laboratory experiments and trial-and-error screening, which are both time-intensive and resource-demanding [10]. With the rapid evolution of computational biology and big data analytics, Artificial Intelligence (AI) has emerged as a transformative force in modern drug discovery. By integrating vast genomic, proteomic, and metabolomic datasets with predictive modeling, AI enables more efficient and precise identification of disease-relevant targets, accelerating the progression from basic research to clinical development [11]. Target identification is a pivotal step in drug discovery, as the accuracy of this stage determines the success of downstream processes. AI algorithms are capable of analyzing complex multi-omics datasets—including genomic, proteomic, transcriptomic, and metabolomic information—to uncover molecular signatures and pathways associated with specific diseases [12]. These data-driven insights allow researchers to pinpoint novel and more precise therapeutic targets. Additionally, deep learning frameworks, exemplified by platforms like *AlphaFold*, have revolutionized structural biology by accurately predicting three-dimensional protein structures and their potential binding sites. This structural

insight provides a strong foundation for rational drug design, enabling the selection of targets with higher clinical relevance and reduced failure rates [13]. Once potential targets are identified, the next crucial step involves the screening of lead compounds that can effectively interact with these targets. Conventional high-throughput screening methods, though effective, require enormous resources and time. AI-based virtual screening and molecular docking approaches significantly accelerate this process by computationally evaluating thousands of compounds for their binding affinity and interaction potential [14-15]. Moreover, machine learning (ML) models enhance this step by predicting crucial ADMET properties—absorption, distribution, metabolism, excretion, and toxicity—early in the development phase. This proactive screening helps in filtering out unsuitable candidates at the very beginning, thereby saving considerable time and cost while increasing the likelihood of clinical success [16-17]. Drug repurposing has gained immense importance in recent years, especially as a strategy to reduce drug development timelines and costs. AI-powered platforms are particularly well-suited for this task as they can systematically analyze existing drug databases to identify off-target effects and uncover new therapeutic indications for approved drugs. By recognizing novel drug–disease associations and molecular mechanisms, AI accelerates the repositioning of existing molecules, bypassing many early-stage development hurdles such as safety assessments and toxicity studies. This not only shortens the time to market but also significantly improves the overall success rate of drug development programs [18-19].Table 1

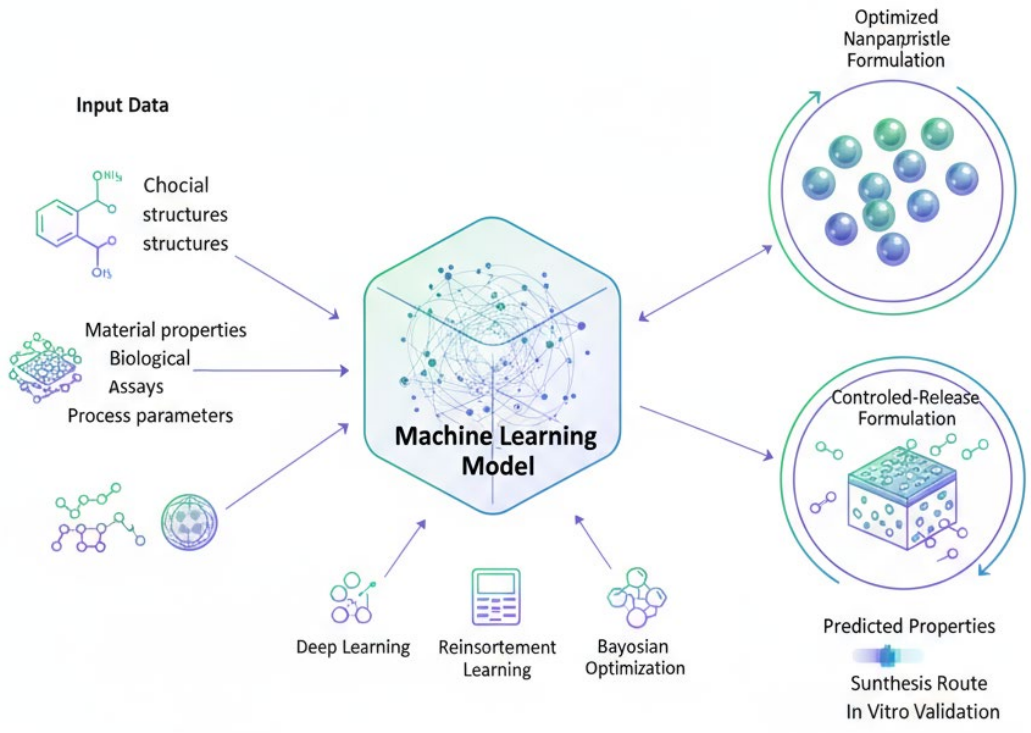
Table 1. AI Applications in Early Drug Discovery

Application	AI Approach	Benefits	Example	Reference
Target identification	Deep learning	High throughput, precise	AlphaFold protein structure prediction	20
Virtual screening	Machine learning	Reduced experimental cost	Predictive ligand docking	21
ADMET prediction	Regression models, ML	Early toxicity avoidance	Liver toxicity prediction models	22
Drug repurposing	Network analysis	Reduced time to clinical trials	AI-based COVID-19 drug repurposing	23

3. AI in Pharmaceutics and Formulation Design

While AI is making significant strides in drug discovery, its impact on pharmaceutics and formulation design is equally transformative. Traditional formulation development is often characterized by an extensive trial-and-error approach, requiring numerous experimental iterations to optimize excipients, delivery systems, and dosage forms. This not only delays the development timeline but also escalates costs. By leveraging machine learning (ML) and advanced predictive analytics, AI streamlines formulation design, improves precision, and personalizes therapeutic strategies [24-25]. Through computational modeling and real-time data integration, AI enables researchers to design more efficient drug delivery systems, enhance stability, and optimize pharmacokinetic–pharmacodynamic (PK/PD) outcomes with remarkable accuracy. Nanotechnology has revolutionized drug delivery by enabling site-specific, controlled, and sustained release of therapeutics [26-27]. However, the design of effective nanocarriers requires fine-tuning multiple parameters such as particle size, surface charge, composition, and functionalization. AI-based algorithms simplify this complex process by predicting optimal nanoparticle characteristics that maximize targeting efficiency and therapeutic outcomes. For example, ML models can analyze vast datasets from previous formulations to suggest the ideal combination of materials and surface modifications for a given drug and disease target [28]. Moreover, the integration of patient-specific data**,** including genetic and physiological profiles, facilitates the development of personalized nanomedicine platforms—ensuring that each formulation is tailored to achieve the best clinical response with minimal adverse effects. Achieving the right balance between drug stability and controlled-release kinetics is a major formulation challenge [29-30]. Traditionally, this involves labor-intensive experimentation with excipients, polymer matrices, and encapsulation methods. AI changes this dynamic by employing machine learning models to optimize excipient selection, polymer ratios, and encapsulation techniques based on predictive patterns rather than trial-and-error [31-32]. By simulating how various formulation parameters influence drug release profiles, AI can identify the most stable and effective combinations before actual laboratory testing. This reduces experimental workload, shortens development cycles, and ensures better reproducibility. Furthermore, predictive models can anticipate stability issues under different storage conditions, helping in the early design of robust and shelf-stable formulations [33-34]. A critical component of successful formulation development is understanding how a drug behaves inside the body—how it is absorbed, distributed, metabolized, and excreted. AI-driven PK/PD (pharmacokinetic/pharmacodynamic) modeling integrates in vitro, in vivo, and clinical data to generate highly accurate simulations of these processes. Such models enable researchers to predict dose–response relationships, optimize dosing regimens, and improve therapeutic efficacy. Importantly, AI-assisted PK/PD models are increasingly being used to support bioequivalence studies, regulatory submissions, and clinical trial design, thereby bridging the gap between bench-scale formulations and real-world clinical outcomes. This approach enhances the predictability of therapeutic performance while minimizing the need for extensive human trials at the early stages [35-36].(Figure 1)

Figure 1. AI-Driven Formulation Development Workflow



4. AI in Clinical Pharmacology

Clinical pharmacology plays a pivotal role in bridging the gap between laboratory discoveries and real-world therapeutic applications. Traditionally, this stage of drug development has been one of the most resource-intensive and uncertain, often involving long timelines, complex clinical trials, and unpredictable patient responses [37-38]. Artificial Intelligence (AI) is now revolutionizing this field by enabling more precise predictions of drug efficacy and safety, optimizing clinical trial design, and enhancing post-marketing surveillance. By analyzing large, multidimensional datasets—ranging from genomic profiles to electronic health records—AI helps personalize treatments, reduce clinical trial failures, and ensure better patient outcomes [39-40]. One of the most transformative impacts of AI in clinical pharmacology is its ability to support personalized medicine. Traditional treatment approaches often adopt a "one-size-fits-all" model, which can lead to suboptimal efficacy and increased adverse drug reactions in patients with unique genetic or physiological characteristics. AI-driven models leverage genetic, phenotypic, and environmental data to predict individual drug responses more accurately [41-42]. This includes pharmacogenomic insights, biomarker analysis, and real-time patient monitoring, allowing clinicians to tailor treatment regimens for each patient. As a result, AI not only improves therapeutic outcomes and patient safety but also reduces the incidence of adverse drug events, enhancing overall treatment effectiveness and patient adherence [43-44].Clinical trials are often plagued by inefficiencies, including challenges in patient recruitment, high dropout rates, and variability in treatment response. These issues can lead to extended timelines and inflated costs.

AI offers a powerful solution by predicting patient recruitment rates, assessing dropout risks, and identifying response variability through advanced statistical modeling and machine learning algorithms. This allows for smarter trial designs, better patient stratification, and more efficient resource allocation. By optimizing inclusion and exclusion criteria, AI enables researchers to conduct more targeted and adaptive clinical trials, ultimately improving the probability of regulatory approval and accelerating the time to market for new therapies [45-46]. Ensuring drug safety is a critical responsibility throughout the lifecycle of a pharmaceutical product. Traditional pharmacovigilance systems rely on voluntary reporting and manual data analysis, which can be slow and limited in scope. AI significantly enhances this process by using natural language processing (NLP) to mine vast and unstructured data sources—including scientific literature, electronic health records (EHRs), spontaneous reporting databases, and even social media platforms—to detect potential adverse drug reactions (ADRs) early and more comprehensively [47-48]. Furthermore, AI-driven signal detection systems can rapidly identify and flag safety concerns, enabling quicker regulatory reporting and intervention. This proactive approach strengthens post-marketing surveillance and enhances patient safety on a global scale [49].(Table 2)

Table 2. AI in Clinical Translation

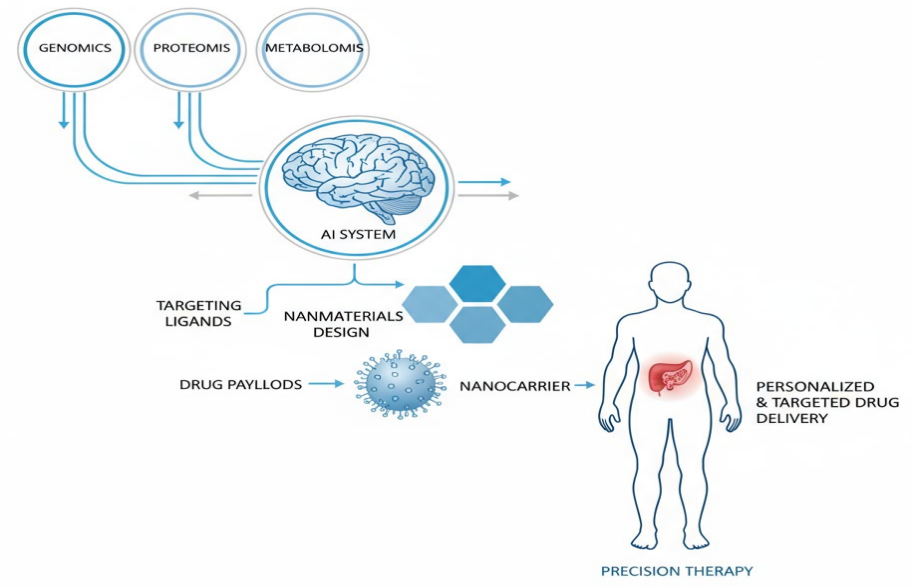
Phase	AI Application	Benefit	Reference
Patient stratification	ML models using genomic and phenotypic data	Personalized therapy, reduced adverse events	50
Trial design	Predictive modeling	Optimized sample size, faster enrollment	51
Safety monitoring	NLP and ML	Early detection of adverse events	52

5. Integration of AI with Multi-Omics and Nanotechnology

The integration of Artificial Intelligence (AI) with multi-omics technologies and nanotechnology represents one of the most promising frontiers in modern biomedical research and drug development [53]. Traditional drug discovery and delivery approaches often rely on isolated datasets and empirical optimization methods, which limit their precision and scalability. In contrast, AI, when combined with the rich layers of biological data generated from multi-omics

platforms and the versatility of nanotechnology-driven delivery systems, enables a far more targeted, personalized, and effective therapeutic approach [54-55]. This convergence not only accelerates the development of novel treatments but also enhances their safety and clinical efficacy.Multi-omics technologies—including genomics, transcriptomics, proteomics, metabolomics, and epigenomics—offer a comprehensive understanding of disease biology at multiple molecular levels. However, the volume and complexity of these datasets make manual interpretation nearly impossible [56-57]. AI algorithms can efficiently process and integrate these high-dimensional datasets, identifying patterns and predicting drug responses, therapeutic efficacy, and potential toxicity with unprecedented accuracy. By correlating omics signatures with clinical outcomes, AI enables researchers to stratify patients into molecular subgroups, paving the way for more personalized and precision-based interventions [58-59]**.** At the same time, nanotechnology-driven delivery systems bring powerful advantages to therapeutic design. Nanocarriers can enhance drug solubility, stability, bioavailability, and target specificity while minimizing systemic side effects. When coupled with AI, these systems become even more powerful: AI models can predict the optimal nanoparticle composition, surface functionalization, and release profile required for precise drug targeting [60-61]. This allows for the rational design of smart nanocarriers that can adapt to individual patient profiles and disease microenvironments, improving overall treatment outcomes.Furthermore, AI plays a critical role in optimizing drug–carrier combinations and dosing regimens for individualized therapy. Through advanced simulation and predictive modeling, AI can assess how different formulations interact with biological systems, enabling personalized dosing strategies that maximize therapeutic efficacy while minimizing toxicity. This synergistic integration of AI, multi-omics, and nanotechnology is laying the foundation for a new era of precision medicine—one where treatments are not only disease-specific but also patient-specific, ensuring better efficacy, safety, and clinical success [62-63].

Figure 2. AI Integration with Multi-Omics and Nanotechnology for Precision Therapy



6. Regulatory, Ethical, and Practical Considerations

The integration of AI into drug discovery and nanotechnology-based therapeutic strategies isn't just a technological revolution—it's also a regulatory, ethical, and logistical balancing act. Despite the rapid pace of innovation, AI-derived predictions must undergo rigorous validation before they can be applied in clinical settings. Current regulatory frameworks, like those from the FDA or EMA, are still catching up to the complexities of AI algorithms, real-time learning systems, and adaptive trial designs [65-66]. A lack of standardized guidelines for evaluating and approving AI-generated outputs can delay clinical translation. Regulatory bodies are pushing for greater algorithmic explainability and robust evidence to ensure patient safety and treatment efficacy.AI in healthcare raises serious ethical questions. Patient data—especially genomic and multi-omics information—is highly sensitive and vulnerable to misuse. Ensuring data privacy, obtaining informed consent, and maintaining transparency in algorithmic decision-making are critical. Moreover, biases embedded in training datasets can lead to unequal or inaccurate treatment recommendations, which could worsen healthcare disparities if not addressed early on.While AI models promise unprecedented precision, their performance depends heavily on the quality, quantity, and diversity of input data [68-69]**.** Many current datasets lack standardization, making reproducibility a major bottleneck. Additionally, the "black box" nature of many AI systems complicates the interpretability of their predictions, often leaving clinicians hesitant to trust or adopt these tools. Overcoming these barriers requires a strong infrastructure for data sharing, explainable AI models, and cross-disciplinary collaboration between researchers, regulators, and healthcare providers [70-71].

7. Future Perspectives

The convergence of artificial intelligence with nanotechnology, pharmacology, and precision medicine is laying the foundation for a transformative era in healthcare. Future directions are expected to address current limitations and unlock new dimensions of innovation and clinical utility [73-74]. One of the most crucial steps forward involves increasing the transparency and interpretability of AI algorithms. XAI frameworks aim to make complex predictive models understandable to clinicians, researchers, and regulatory authorities. This not only enhances trust and accountability but also facilitates regulatory approval and clinical adoption [75-76]. By revealing how AI arrives at specific predictions—such as optimal drug dosages, carrier selection, or toxicity risks—XAI can help bridge the gap between data science and practical medicine. The future of therapeutics lies in multi-modal strategies that combine pharmacological interventions with gene therapy, nanomedicine, and advanced biomaterials [77-78]. AI can integrate these diverse therapeutic modalities, optimizing treatment protocols for synergistic effects and personalized outcomes. This integrative approach has the potential to improve therapeutic efficacy, minimize adverse reactions, and accelerate the path from preclinical research to real-world application.AI-powered systems are evolving from static predictive models to real-time, adaptive monitoring platforms. These can track a patient's physiological responses, drug metabolism, and biomarkers continuously, allowing dynamic adjustment of dosing regimens and formulations. Such systems could significantly reduce the incidence of adverse drug reactions and improve treatment

outcomes through precision feedback loops [79-80].The establishment of collaborative, cloud-based AI ecosystems will revolutionize how drug discovery and development are conducted. By enabling secure sharing of multi-omics datasets, molecular models, and clinical trial outcomes across institutions worldwide, these platforms can accelerate innovation and democratize access to advanced drug development tools. This global synergy will help overcome data silos and foster a more inclusive, efficient, and equitable pharmaceutical research landscape .

8. Conclusion

Artificial Intelligence (AI) is rapidly transforming the landscape of pharmacology and pharmaceutics, offering unprecedented opportunities to accelerate drug discovery, optimize formulations, and enable precision medicine. By leveraging predictive modeling, machine learning, and deep learning techniques, AI significantly reduces development timelines, improves therapeutic efficacy, and facilitates patient-specific treatment strategies. Its integration with nanotechnology enhances targeted and controlled drug delivery, while the incorporation of multi-omics data provides deeper insights into disease mechanisms, drug responses, and toxicity prediction. Moreover, AI-driven clinical pharmacology tools improve trial design, patient stratification, and post-marketing pharmacovigilance, bridging the gap between laboratory research and real-world therapeutic applications.Despite these remarkable advances, several challenges remain. Regulatory frameworks must evolve to address AI-derived predictions, while concerns related to data quality, reproducibility, algorithmic transparency, and ethical use of sensitive patient information require ongoing attention. Nonetheless, the convergence of AI with advanced computational, molecular, and clinical technologies holds immense promise for redefining patient-centered therapeutics. As these tools mature, they are poised to not only streamline the drug development process but also enable more effective, safe, and personalized treatments, ultimately transforming the future of healthcare.

References

1. Deng, J., Yang, Z., Ojima, I., Samaras, D., & Wang, F. (2021). Artificial intelligence in drug discovery: Applications and techniques. *Briefings in Bioinformatics, 23*, bbab430. https://doi.org/10.1093/bib/bbab430
2. Kaul, V., Enslin, S., & Gross, S. A. (2020). History of artificial intelligence in medicine. *Gastrointestinal Endoscopy, 92*, 807–812. https://doi.org/10.1016/j.gie.2020.05.034
3. Hosny, A., Parmar, C., Quackenbush, J., Schwartz, L. H., & Aerts, H. J. (2018). Artificial intelligence in radiology. *Nature Reviews Cancer, 18*, 500–510. https://doi.org/10.1038/s41568-018-0016-5
4. Denecke, K., & Baudoin, C. R. (2022). A review of artificial intelligence and robotics in transformed health ecosystems. *Frontiers in Medicine, 9*, 795957. https://doi.org/10.3389/fmed.2022.795957
5. Paul, D., Sanap, G., Shenoy, S., Kalyane, D., Kalia, K., & Tekade, R. K. (2021). Artificial intelligence in drug discovery and development. *Drug Discovery Today, 26*, 80–93. https://doi.org/10.1016/j.drudis.2020.10.010

6. Wang, L., Ding, J., Pan, L., Cao, D., Jiang, H., & Ding, X. (2019). Artificial intelligence facilitates drug design in the big data era. *Chemometrics and Intelligent Laboratory Systems, 194*, 103850. https://doi.org/10.1016/j.chemolab.2019.103850
7. Grzybowski, A., Pawlikowska-Łagód, K., & Lambert, W. C. (2024). A history of artificial intelligence. *Clinical Dermatology, 42*, 221–229. https://doi.org/10.1016/j.clindermatol.2023.12.001
8. Bredt, S. (2019). Artificial intelligence (AI) in the financial sector—Potential and public strategies. *Frontiers in Artificial Intelligence, 2*, 16. https://doi.org/10.3389/frai.2019.00016
9. Stahl, B. C., Antoniou, J., Ryan, M., Macnish, K., & Jiya, T. (2022). Organisational responses to the ethical issues of artificial intelligence. *AI & Society, 37*, 23–37. https://doi.org/10.1007/s00146-021-01277-x
10. Theodosiou, A. A., & Read, R. C. (2023). Artificial intelligence, machine learning and deep learning: Potential resources for the infection clinician. *Journal of Infection, 87*, 287–294. https://doi.org/10.1016/j.jinf.2023.05.015
11. Gawehn, E., Hiss, J. A., & Schneider, G. (2016). Deep learning in drug discovery. *Molecular Informatics, 35*, 3–14. https://doi.org/10.1002/minf.201501008
12. Mak, K.-K., & Pichika, M. R. (2019). Artificial intelligence in drug development: Present status and future prospects. *Drug Discovery Today, 24*, 773–780. https://doi.org/10.1016/j.drudis.2019.01.020
13. Vora, L. K., Gholap, A. D., Jetha, K., Thakur, R. R. S., Solanki, H. K., & Chavda, V. P. (2023). Artificial intelligence in pharmaceutical technology and drug delivery design. *Pharmaceutics, 15*, 1916. https://doi.org/10.3390/pharmaceutics15081916
14. Choi, R. Y., Coyner, A. S., Kalpathy-Cramer, J., Chiang, M. F., & Campbell, J. P. (2020). Introduction to machine learning, neural networks, and deep learning. *Translational Vision Science & Technology, 9*, 14. https://doi.org/10.1167/tvst.9.2.14
15. Cabrera, A., Bouterse, A., Nelson, M., Razzouk, J., Ramos, O., Chung, D., et al. (2023). Use of the random forest machine learning algorithm to predict short-term outcomes following posterior cervical decompression with instrumented fusion. *Journal of Clinical Neuroscience, 107*, 167–171. https://doi.org/10.1016/j.jocn.2023.03.011
16. Rebollo, R., Oyoun, F., Corvis, Y., El-Hammadi, M. M., Saubamea, B., Andrieux, K., et al. (2022). Microfluidic manufacturing of liposomes: Development and optimization by design of experiment and machine learning. *ACS Applied Materials & Interfaces, 14*, 39736–39745. https://doi.org/10.1021/acsami.2c11122
17. Lin, E., Lin, C.-H., & Lane, H.-Y. (2022). De novo peptide and protein design using generative adversarial networks: An update. *Journal of Chemical Information and Modeling, 62*, 761–774. https://doi.org/10.1021/acs.jcim.1c01529
18. Gupta, R. R. (2022). Application of artificial intelligence and machine learning in drug discovery. In A. Heifetz (Ed.), *Artificial Intelligence in Drug Design* (pp. 113–124). Springer. https://doi.org/10.1007/978-1-0716-2334-5_8
19. Svensson, H. G., Tyrchan, C., Engkvist, O., & Chehreghani, M. H. (2024). Utilizing reinforcement learning for de novo drug design. *Machine Learning, 113*, 4811–4843. https://doi.org/10.1007/s10994-024-06415-x

20. Pearson, G. S. (2024). Artificial intelligence and publication ethics. *Journal of the American Psychiatric Nurses Association, 30*, 453–455. https://doi.org/10.1177/1078390324123456
21. Rogers, W. A., Draper, H., & Carter, S. M. (2021). Evaluation of artificial intelligence clinical applications: Detailed case analyses show the value of healthcare ethics approach in identifying patient care issues. *Bioethics, 35*, 623–633. https://doi.org/10.1111/bioe.12873
22. Nagarajan, N., Yapp, E. K. Y., Le, N. Q. K., Kamaraj, B., Al-Subaie, A. M., & Yeh, H.-Y. (2019). Application of computational biology and artificial intelligence technologies in cancer precision drug discovery. *BioMed Research International, 2019*, 8427042. https://doi.org/10.1155/2019/8427042
23. Zhang, Y., Luo, M., Wu, P., Wu, S., Lee, T.-Y., & Bai, C. (2022). Application of computational biology and artificial intelligence in drug design. *International Journal of Molecular Sciences, 23*, 13568. https://doi.org/10.3390/ijms232113568
24. Deore, A. B., Dhumane, J. R., Wagh, R., & Sonawane, R. (2019). The stages of the drug discovery and development process. *Asian Journal of Pharmaceutical Research and Development, 7*, 62–67. https://doi.org/10.22270/ajprd.v7i4.680
25. Parvathaneni, V., Kulkarni, N. S., Muth, A., & Gupta, V. (2019). Drug repurposing: A promising tool to accelerate the drug discovery process. *Drug Discovery Today, 24*, 2076–2085. https://doi.org/10.1016/j.drudis.2019.05.014
26. Dana, D., Gadhiya, S. V., St. Surin, L. G., Li, D., Naaz, F., Ali, Q., et al. (2018). Deep learning in drug discovery and medicine: scratching the surface. *Molecules, 23*, 2384. https://doi.org/10.3390/molecules23122384
27. Sarkar, C., Das, B., Rawat, V. S., Wahlang, J. B., Nongpiur, A., Tiewsoh, I., et al. (2023). Artificial intelligence and machine learning technology are driving modern drug discovery and development. *International Journal of Molecular Sciences, 24*, 2026. https://doi.org/10.3390/ijms24032026
28. Ciallella, H. L., & Zhu, H. (2019). Advancing computational toxicology in the big data era by artificial intelligence: Data-driven and mechanism-driven modeling for chemical toxicity. *Chemical Research in Toxicology, 32*, 536–547. https://doi.org/10.1021/acs.chemrestox.8b00363
29. Parvatikar, P. P., Patil, S., Khaparkhuntikar, K., Patil, S., Singh, P. K., Sahana, R., et al. (2023). Artificial intelligence: Machine learning approach for screening large databases and drug discovery. *Antiviral Research, 220*, 105740. https://doi.org/10.1016/j.antiviral.2023.105740
30. Singh, S., Gupta, H., Sharma, P., & Sahi, S. (2024). Advances in artificial intelligence (AI)-assisted approaches in drug screening. *Artificial Intelligence in Chemistry, 2*, 100039. https://doi.org/10.1016/j.aic.2024.100039
31. Spanakis, M., Tzamali, E., Tzedakis, G., Koumpouzi, C., Pediaditis, M., Tsatsakis, A., & Sakkalis, V. (2025). Artificial intelligence models and tools for the assessment of drug–herb interactions. *Pharmaceuticals, 18*, 282. https://doi.org/10.3390/ph18040282

32. Li, X., Liang, J., Hu, J., Ma, L., Yang, J., Zhang, A., et al. (2024). Screening for primary aldosteronism on and off interfering medications. *Endocrine, 83*, 178–187. https://doi.org/10.1007/s12020-024-03520-8
33. Rocco, P., Musazzi, U. M., Franzè, S., & Minghetti, P. (2019). Copies of nonbiological complex drugs: Generic, hybrid, or biosimilar? *Drug Discovery Today, 24*, 250–255. https://doi.org/10.1016/j.drudis.2018.10.006
34. Zagalo, D. M., Sousa, J., & Simões, S. (2022). Quality by design (QbD) approach in marketing authorization procedures of non-biological complex drugs: A critical evaluation. *European Journal of Pharmaceutics and Biopharmaceutics, 178*, 1–24. https://doi.org/10.1016/j.ejpb.2022.03.003
35. Saha, E., Rathore, P., Parida, R., & Rana, N. P. (2022). The interplay of emerging technologies in pharmaceutical supply chain performance: An empirical investigation for the rise of Pharma 4.0. *Technological Forecasting and Social Change, 181*, 121768. https://doi.org/10.1016/j.techfore.2022.121768
36. Malheiro, V., Duarte, J., Veiga, F., & Mascarenhas-Melo, F. (2023). Exploiting Pharma 4.0 technologies in the non-biological complex drugs manufacturing: Innovations and implications. *Pharmaceutics, 15*, 2545. https://doi.org/10.3390/pharmaceutics15112545
37. Chan, H. C. S., Shan, H., Dahoun, T., Vogel, H., & Yuan, S. (2019). Advancing drug discovery via artificial intelligence. *Trends in Pharmacological Sciences, 40*, 592–604. https://doi.org/10.1016/j.tips.2019.06.004
38. Shiammala, P. N., Duraimutharasan, N. K. B., Vaseeharan, B., Alothaim, A. S., Al-Malki, E. S., Snekaa, B., et al. (2023). Exploring the artificial intelligence and machine learning models in the context of drug design difficulties and future potential for the pharmaceutical sectors. *Methods, 219*, 82–94. https://doi.org/10.1016/j.ymeth.2023.02.005
39. Singh, S., Kaur, N., & Gehlot, A. (2024). Application of artificial intelligence in drug design: A review. *Computers in Biology and Medicine, 179*, 108810. https://doi.org/10.1016/j.compbiomed.2024.108810
40. Rashid, M. B. M. A. (2021). Artificial intelligence is affecting a paradigm shift in drug development. *SLAS Technology, 26*, 3–15. https://doi.org/10.1177/2472630320964785
41. Doytchinova, I. (2022). Drug design—Past, present, future. *Molecules, 27*, 1496. https://doi.org/10.3390/molecules27051496
42. Gholap, A. D., Uddin, J., Faiyazuddin, Omri, A., Gowri, S., & Khalid, M. (2024). Advances in artificial intelligence for drug delivery and development: A comprehensive review. *Computers in Biology and Medicine, 178*, 108702. https://doi.org/10.1016/j.compbiomed.2024.108702
43. Jumper, J., Evans, R., Pritzel, A., Green, T., Figurnov, M., Ronneberger, O., Tunyasuvunakool, K., Bates, R., Žídek, A., Potapenko, A., et al. (2021). Highly accurate protein structure prediction with AlphaFold. *Nature, 596*, 583–589. https://doi.org/10.1038/s41586-021-03819-2

44. Hu, W., & Ohue, M. (2024). SpatialPPI: Three-dimensional space protein-protein interaction prediction with AlphaFold Multimer. *Computational and Structural Biotechnology Journal, 23*, 1214–1225. https://doi.org/10.1016/j.csbj.2025.01.001
45. Ahmed, F., Samantasinghar, A., Soomro, A. M., Kim, S., & Choi, K. H. (2023). A systematic review of computational approaches to understand cancer biology for informed drug repurposing. *Journal of Biomedical Informatics, 142*, 104373. https://doi.org/10.1016/j.jbi.2023.104373
46. Park, K. (2019). A review of computational drug repurposing. *Translational and Clinical Pharmacology, 27*, 59–63. https://doi.org/10.12793/tcp.2019.27.2.59
47. Issa, N. T., Stathias, V., Schürer, S., & Dakshanamurthy, S. (2021). Machine and deep learning approaches for cancer drug repurposing. *Seminars in Cancer Biology, 68*, 132–142. https://doi.org/10.1016/j.semcancer.2020.07.003
48. Bajorath, J. (2024). Origins and progression of the polypharmacology concept in drug discovery. *Artificial Intelligence in Life Sciences, 5*, 100094. https://doi.org/10.1016/j.ailsci.2024.100094
49. Cichońska, A., Ravikumar, B., & Rahman, R. (2024). AI for targeted polypharmacology: The next frontier in drug discovery. *Current Opinion in Structural Biology, 84*, 102771. https://doi.org/10.1016/j.sbi.2024.102771
50. Raman, K., Kumar, R., Musante, C. J., & Madhavan, S. (2025). Integrating model-informed drug development with AI: A synergistic approach to accelerating pharmaceutical innovation. *Clinical and Translational Science, 18*, e70124. https://doi.org/10.1111/cts.70124
51. Peters, S. A. (2021). Applications of physiologically based pharmacokinetic models integrated with drug effect models (PBPK/PD). In *Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulations: Principles, Methods, and Applications in the Pharmaceutical Industry* (2nd ed., pp. 353–374). John Wiley & Sons. https://doi.org/10.1002/9781119815079.ch14
52. Saeheng, T., Karbwang, J., & Na-Bangchang, K. (2024). Population-pharmacokinetic/pharmacodynamic model of Atractylodes lancea (Thunb.) DC. administration in patients with advanced-stage intrahepatic cholangiocarcinoma: A dosage prediction. *BMC Complementary Medicine and Therapies, 24*, 384. https://doi.org/10.1186/s12906-024-04384-1
53. Chou, W.-C., Chen, Q., Yuan, L., Cheng, Y.-H., He, C., Monteiro-Riviere, N. A., Riviere, J. E., & Lin, Z. (2023). An artificial intelligence-assisted physiologically-based pharmacokinetic model to predict nanoparticle delivery to tumors in mice. *Journal of Controlled Release, 361*, 53–63. https://doi.org/10.1016/j.jconrel.2023.03.001
54. Chou, W.-C., & Lin, Z. (2022). Machine learning and artificial intelligence in physiologically based pharmacokinetic modeling. *Toxicological Sciences, 191*, 1–14. https://doi.org/10.1093/toxsci/kfac090
55. Li, Y., Wang, Z., Li, Y., Du, J., Gao, X., Li, Y., & Lai, L. (2024). A combination of machine learning and PBPK modeling approach for pharmacokinetics prediction of small molecules in humans. *Pharmaceutical Research, 41*, 1369–1379. https://doi.org/10.1007/s11095-024-03567-3

56. Wu, K., Li, X., Zhou, Z., Zhao, Y., Su, M., Cheng, Z., Wu, X., Huang, Z., Jin, X., Li, J., et al. (2024). Predicting pharmacodynamic effects through early drug discovery with artificial intelligence-physiologically based pharmacokinetic (AI-PBPK) modelling. *Frontiers in Pharmacology, 15*, 1330855. https://doi.org/10.3389/fphar.2024.1330855
57. Umscheid, C. A., Margolis, D. J., & Grossman, C. E. (2011). Key concepts of clinical trials: A narrative review. *Postgraduate Medicine, 123*, 194–204. https://doi.org/10.3810/pgm.2011.11.2486
58. Fogel, D. B. (2018). Factors associated with clinical trials that fail and opportunities for improving the likelihood of success: A review. *Contemporary Clinical Trials Communications, 11*, 156–164. https://doi.org/10.1016/j.conctc.2018.08.001
59. Cunningham, J. W., Abraham, W. T., Bhatt, A. S., Dunn, J., Felker, G. M., Jain, S. S., et al. (2024). Artificial intelligence in cardiovascular clinical trials. *Journal of the American College of Cardiology, 84*, 2051–2062. https://doi.org/10.1016/j.jacc.2024.03.002
60. Chopra, H., Annu, Kil Shin, D., Munjal, K., Priyanka, & Dhama, K., Bin Emran, T. (2023). Revolutionizing clinical trials: The role of AI in accelerating medical breakthroughs. *International Journal of Surgery, 109*, 4211–4220. https://doi.org/10.1016/j.ijsu.2023.04.014
61. Zhang, Y., Mastouri, M., & Zhang, Y. (2024). Accelerating drug discovery, development, and clinical trials by artificial intelligence. *Medicine, 5*, 1050–1070. https://doi.org/10.1016/j.med.2024.08.005
62. Goldberg, J. M., Amin, N. P., Zachariah, K. A., & Bhatt, A. B. (2024). The introduction of AI into decentralized clinical trials. *JACC: Advances, 3*, 101094. https://doi.org/10.1016/j.jacadv.2024.101094
63. Lu, X., Yang, C., Liang, L., Hu, G., Zhong, Z., & Jiang, Z. (2024). Artificial intelligence for optimizing recruitment and retention in clinical trials: A scoping review. *Journal of the American Medical Informatics Association, 31*, 2749–2759. https://doi.org/10.1093/jamia/ocad101
64. Fountzilas, E., Tsimberidou, A. M., Vo, H. H., & Kurzrock, R. (2022). Clinical trial design in the era of precision medicine. *Genome Medicine, 14*, 101. https://doi.org/10.1186/s13073-022-01110-8
65. Jayatunga, M. K., Ayers, M., Bruens, L., & Jayanth, D., Meier, C. (2024). How successful are AI-discovered drugs in clinical trials? A first analysis and emerging lessons. *Drug Discovery Today, 29*, 104009. https://doi.org/10.1016/j.drudis.2024.104009
66. Chen, H., Engkvist, O., Wang, Y., Olivecrona, M., & Blaschke, T. (2018). The rise of deep learning in drug discovery. *Drug Discovery Today, 23*, 1241–1250. https://doi.org/10.1016/j.drudis.2018.01.039
67. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., et al. (2019). Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery, 18*, 463–477. https://doi.org/10.1038/s41573-019-0024-5

68. Stokes, J. M., Yang, K., Swanson, K., Jin, W., Cubillos-Ruiz, A., Donghia, N. M., et al. (2020). A deep learning approach to antibiotic discovery. *Cell, 180*, 688–702. https://doi.org/10.1016/j.cell.2020.01.021
69. Mamoshina, P., Vieira, A., Putin, E., & Zhavoronkov, A. (2016). Applications of deep learning in biomedicine. *Molecular Pharmaceutics, 13*, 1445–1454. https://doi.org/10.1021/acs.molpharmaceut.5b00982
70. Vamathevan, J., Clark, D., Czodrowski, P., Dunham, I., Ferran, E., Lee, G., Li, B., Madabhushi, A., Shah, P., Spitzer, M., et al. (2019). Applications of machine learning in drug discovery and development. *Nature Reviews Drug Discovery, 18*, 463–477. https://doi.org/10.1038/s41573-019-0024-5
71. Ekins, S., Puhl, A. C., Zorn, K. M., Lane, T. R., Russo, D. P., Klein, J. J., Hickey, A. J., & Clark, A. M. (2019). Exploiting machine learning for end-to-end drug discovery and development. *Nature Materials, 18*, 435–441. https://doi.org/10.1038/s41563-019-0338-0
72. Lavecchia, A. (2019). Deep learning in drug discovery: Opportunities, challenges and future prospects. *Drug Discovery Today, 24*, 2017–2032. https://doi.org/10.1016/j.drudis.2019.05.018
73. Walters, W. P., Murcko, M., & Murcko, M. A. (2020). Assessing the impact of generative AI on medicinal chemistry. *Nature Biotechnology, 38*, 143–145. https://doi.org/10.1038/s41587-019-0396-1
74. Elton, D. C., Boukouvalas, Z., Fuge, M. D., & Chung, P. W. (2019). Deep learning for molecular design—a review of the state of the art. *Molecular Systems Design & Engineering, 4*, 828–849. https://doi.org/10.1039/C9ME00039A
75. Chen, H., Engkvist, O., Wang, Y., Olivecrona, M., & Blaschke, T. (2018). The rise of deep learning in drug discovery. *Drug Discovery Today, 23*, 1241–1250. https://doi.org/10.1016/j.drudis.2018.01.039
76. Stokes, J. M., Yang, K., Swanson, K., Jin, W., Cubillos-Ruiz, A., Donghia, N. M., et al. (2020). A deep learning approach to antibiotic discovery. *Cell, 180*, 688–702. https://doi.org/10.1016/j.cell.2020.01.021
77. Mamoshina, P., Vieira, A., Putin, E., & Zhavoronkov, A. (2016). Applications of deep learning in biomedicine. *Molecular Pharmaceutics, 13*, 1445–1454. https://doi.org/10.1021/acs.molpharmaceut.5b00982
78. Schneider, G. (2018). Automating drug discovery. *Nature Reviews Drug Discovery, 17*, 97–113. https://doi.org/10.1038/nrd.2017.232
79. Chen, H., Engkvist, O., Wang, Y., Olivecrona, M., & Blaschke, T. (2018). The rise of deep learning in drug discovery. *Drug Discovery Today, 23*, 1241–1250. https://doi.org/10.1016/j.drudis.2018.01.039
80. Walters, W. P., Murcko, M., & Murcko, M. A. (2020). Assessing the impact of generative AI on medicinal chemistry. *Nature Biotechnology, 38*, 143–145. https://doi.org/10.1038/s41587-019-0396-1