STM JOURNALS

Research & Reviews: A Journal of
Drug Design & Discovery

ISSN: 2349-9036
Volume 12, Issue 2, 2025
May–August
DOI (Journal): 10.37591/RRJoDDD

https://journals.stmjournals.com/rrjoddd

Research RRJoDDD

Accelerating Drug Discovery with AI: Transforming the Pharmaceutical Pipeline

Aditya P. Singh[1], Akanksha Dwivedi[2,*], G. N. Darwhekar[3]

Abstract

The revolutionary potential of artificial intelligence (AI) is examined in this essay by the pharmaceutical industry, highlighting its application across the drug development lifecycle. AI, specifically via deep learning models and machine learning (ML), such as GANs, RNNs, and transformers, enhances drug discovery, formulation, toxicity prediction, and clinical trials. It streamlines processes, like identification of targets, virtual screening, modeling of structure-activity relationships, and medication repurposing. AI is also employed in optimizing formulations for controlled and immediate release tablets, capsules, and advanced drug delivery systems. Despite its possibilities, obstacles, like data availability, model interpretability, and lack of clinical expertise remain. The article concludes that AI has already demonstrated significant impact in pharmaceutical R&D and is poised to further revolutionize personalized medicine, improve patient outcomes, and accelerate innovation in the sector.

Keywords: Artificial intelligence, machine learning, drug discovery, formulation challenge, AI in pharmaceutical business

INTRODUCTION

"Artificial Intelligence" (AI) refers to the least degree of human involvement that may be achieved when a computer simulates intelligent action. AI is the computer science field that emphasizes on programming that solves problems [1]. AI possesses distinct qualities that provide it the ability to act and think in ways that maximize the likelihood of reaching a destination. AI does this by using a range of algorithms that simulate even the most fundamental human cognitive abilities.

AI is currently becoming more popular across several industries, with the pharmaceutical sector leading the way. Response surface analysis is one statistical technique that formulators have historically favored method for design space analysis. This research underscores the useful applications AI in pharmaceutical production, including drug R&D, drug repurposing, boosting pharmaceutical manufacturing, clinical trials, etc. The medication research process is accelerated by these apps, which also reduce the requirement for human labor [2]. In recent years, there has been a major advancement in the digitization of data in the pharmaceutical manufacturing business.

***Author for Correspondence**
Akanksha Dwivedi
E-mail id: akd.pharma@gmail.com

[1]Student, Department of Pharmaceutics, Acropolis Institute of Pharmaceutical Education and Research, Indore, Madhya Pradesh, India.
[2]Associate Professor, Department of Pharmaceutics, Acropolis Institute of Pharmaceutical Education and Research, Indore, Madhya Pradesh, India.
[3]Principal, Department of Pharmacy, Acropolis Institute of Pharmaceutical Education and Research, Indore, Madhya Pradesh, India.

Submission Date: June 08, 2025
Acceptance Date: June 26, 2025
Published Date: August,01,2025

Citation: Aditya P. Singh, Akanksha Dwivedi, G. N. Darwhekar. Accelerating Drug Discovery with AI: Transforming the Pharmaceutical Pipeline. Research & Reviews: A Journal of Drug Design & Discovery. 2025; 12(2): 77–84p.

Rapid advancements in AI-guided automation, according to the McKinsey Global Institute would profoundly change how society perceives work [3]. AI may be used to increase the effectiveness of pharmaceutical products at every stage of their life cycle, which includes finding new drugs, improving existing ones, creating new formulations, characterizing them, testing their quality, marketing

them, and monitoring them after they are sold.

Notwithstanding the encouraging developments, there are still difficulties in incorporating AI into pharmaceutical procedures. Significant obstacles to broad adoption include problems, like data heterogeneity, difficulties integration, and the requirement for specialized expertise.

There are two types of learning: Both unsupervised and supervised learning (SL) are possible. In unsupervised learning, incoming data is fed into the network, which scans it for patterns or structures and condenses it into a more manageable format [4]. Artificial neurones analyze input and produce a result that is transmitted to the subsequent perception.

TOOLS, TECHNOLOGY, AND NETWORKS

One important subfield of AI, is machine learning (ML). One important aspect of ML is in-depth instruction, which makes use of artificial neural network (ANN). The ANN is made up of multilayer functional units. By mimicking the way electrical impulses go through the brain, it replicates the functioning of the human brain. Biological factors are the main drivers of these systems. It receives input and learns directly from it; fundamentally, neurons express an output by summing up all the information (Table 1) [5].

Table 1. The top ten AI models used most often in the pharmaceutical business [6–9].

AI and Machine Learning Models	Overview/Use
GANs, or Making Adversarial Networks	In the manufacturing of pharmaceutical items, GANs are widely used to generate new chemical compounds and improve existing properties. A discriminator network is used with GANs to create architecturally diverse and functionally optimized drug candidates to assess the quality of the novel molecules produced by the generator network.
Repeated Neural Networks (RNNs)	RNNs are widely utilized for sequence-based activities in drug development such peptide sequence design, genetic data analysis, and protein structure prediction. They record sequential relationships and has the ability to create new sequences using patterns it has learnt.
Reinforcement Learning (RL)	Personalized treatment regimens and drug dosage optimization have been achieved using RL methods. To make sequential judgments that help with dose optimization and enhance patient outcomes, RL algorithms pick up knowledge through interactions with their surroundings.
Transformer Models	Transformer models have been applied to natural language processing jobs in the pharmaceutical sector, such as the well-known BERT (Bidirectional Encoder Representations from Transformers) model. They can extract valuable data from clinical trials, patent databases, and scientific literature that helps researchers make well-informed judgments about medication development.

PRODUCT LIFE CYCLE FOR PHARMACEUTICALS

AI can assist in decision-making, facilitate the creation of rational drugs, choose the most effective way to treat a patient using customized drugs, complete the clinical data generated, then used that data to develop future medications [10]. It makes sense to believe that AI will help create pharmaceutical items between the laboratory and the patient's bed.

UTILIZING AI IN DRUG DISCOVERY

In many respects, AI has transformed drug development and discovery. The following are a few of AI's major contributions in this field.

Identifying the Target

AI systems can analyze a range of data sources, including clinical, proteomic, and genomic data, to identify potential therapeutic targets. By discovering targets and molecular pathways associated with disease, AI helps design medications that can change biological processes.

Virtual Screening

AI enables the effective screening of vast chemical libraries to identify potential treatment candidates that have a high probability of attaching to a particular target. Through the modelling of chemical interactions and the prediction of binding affinities, AI helps researchers prioritize and choose compounds for experimental testing, saving them time and money.

Structural Activity Relationship (SAR) Modelling

Models of AI can correlate a molecule's chemical makeup with its biological activity. To maximize therapeutic potential, scientists can use this to design molecules with desired features, including high potency, selectivity, and attractive pharmacokinetic profiles.

Optimizing Potential Drugs

By considering several factors, including pharmacokinetics, safety, and efficacy, AI systems may assess and enhance drug candidates. This helps researchers optimize medicinal substances to enhance effectiveness and minimize side effects.

Reusing Drugs

AI techniques can be used to examine large amounts of biomedical data and identify existing drugs that could be helpful in treating a range of diseases. AI speeds up the drug discovery process and lowers costs by repurposing current medications for new use.

Forecast of Toxicity

AI systems can predict the toxicity of medications by analyzing the chemical structure and properties of molecules. ML algorithms can identify hazardous structural traits or forecast unfavorable outcomes after being trained on toxicological databases. This aids scientists in prioritizing safer compounds and reducing the possibility of negative clinical trial reactions.

All things considered, in drug research and development, AI-driven techniques could streamline and speed up identifying, enhancing, and creating novel therapeutic candidates, ultimately leading to more potent and efficient medications. Pharmaceutical companies, for instance, employ using *in silico* target fishing technology (TF) to predict biological targets using chemical structure. This information is given in accordance with Information with biological annotations in the chemical database. Moreover, several other methods were used to acquire target class information required for effective planning and explore the mechanism of action, such as data mining and chemical structure docking [11]. The typical drug discovery procedures that are employed by many industries are somewhat costly since they require several complex steps that must be properly addressed to be finished, such as the meticulous identification and selection of target proteins and the thorough mechanism of action of small molecules. The overall experimental cost throughout the drug development procedures was reduced by using TF to speed up this process. The ligand-target is predicted by using reference molecules and the 3D descriptors.

Table 2. Typical AI model methods for drug discovery.

AI Models Tools	Summary
Deep Chem	Among the various tools and models for drug discovery provided by this open-source toolbox are deep learning models for generative chemistry, virtual screening, and molecular property prediction.
RDKit	An open-source cheminformatics library that is widely used and has several capabilities for handling molecules, determining substructures, and computing descriptors. In drug discovery applications, it can be integrated with machine learning frameworks.
Graph Conv	An architecture for deep learning models based on molecular graphs. Molecular properties, such as toxicity and bioactivity have been successfully predicted by utilizing the structural information found in the graph representation of molecules.

Drug development has advanced significantly because of the use of AI models and methodologies. Some of the most popular AI model tools for drug discovery are included in Table 2. These and other AI model strategies are available for drug discovery. New models and methods are constantly being developed to speed up discovering new drugs, as the sector is undergoing rapid change.

AI IN DRUG DEVELOPMENT & FORMULATION

A distinct medicinal component must then be included in an acceptable dose form with the required features for delivery. In this instance, AI can take the role of the traditional trial-and-error method [12]. Numerous computational methods, including QSPR, may be able to address formulation design issues, including porosity, dissolution, instability, and many more [13].

To achieve the required dissolving profile, Piroxicam direct-filling hard gelatin capsules were developed using a hybrid methodology that blends ANN with expert systems (ES). The Model Expert System offers formulation development recommendations and judgments based on the parameters that are presented. On the other hand, ANNs provide trouble-free formulation construction by connecting the formulation parameters to the back propagation learning intended result. This procedure is cooperatively managed by the control module.

In addition to standard dosage forms, pharmaceutical sciences have seen the emergence of other formulations, For instance, liposomes, extrudates, pellets, solid dispersions, and nanoparticles. These methods are referred described as “formulation techniques” since they empower creating new formulations or adding functionality to standard dose forms, like tablets. Because AI applications in formulation approaches are even more valuable to study to create next-generation therapeutic products with the intended efficacy and health outcomes. These methods can effectively address several API issues, including poor manufacturing capability, stability, bioavailability, and solubility [14].

a) *Controlled release tablets formulation:* To create controlled-release formulations, researchers employ ANN and pharmacokinetic simulations. Using Chem software, the input and output data units teach the ANN model sophisticated and specialized skills. To predict the optimal tablet formulations, researchers employ a complex ANN model based on two ideal *in vitro* dissolving time profiles and two desired *in vivo* release profiles. Since dissolution is linearly correlated with the amount of medicine taken *in vivo*, it is the rate-limiting step in the medication’s *in vivo* absorption. The similarity factor (f2) and difference factor (f1) are frequently used to identify *in vitro* release patterns [15].
b) *Immediate-release tablet formulation:* Turkoglu created a direct compression tablet formulation with hydrochlorothiazide to increase tablet strength [16]. To explain the diluting agent and binder content in each formulation, as well as the characteristics of granules and tablets and processing variables (granulator type and technique), Kesavan and Peck developed a model of a caffeine tablet formulation in a different study on adding binder.
c) *Formulation of hard gelatin capsule shells:* Executive techniques, such as ES and ANN, are employed in the creation of hard gelatin capsule formulations. ANNs’ domain expertise stimulates human brain processes, like learning, generalization, abstraction, and prediction. The statistics and data gathered during an inquiry activity can be swiftly converted into knowledge. Utilizing ANNs, giving the creator the ability to predict the characteristics of the theoretical preparation or create a few domain-specific strategies for upcoming occasions [17]. By growing the Expert Network and doing analysis, Wendy I. Wilson created a capsule shell manufacturing process in 2005 for drugs included in the Biopharmaceutical Classification System II, such as ibuprofen, carbamazepine, ketoprofen, and naproxen. Despite the drawback of simply providing a recommended composition.
d) *Other formulation techniques:* Researchers have also used AI techniques on colloidal systems, micelles, beads and pellets, microparticles and nanoparticles, microspheres and nanospheres, liposomes and nanoliposomes, and liquid and solid dosage forms in addition to these formulation techniques (Figure 1) [18–20].

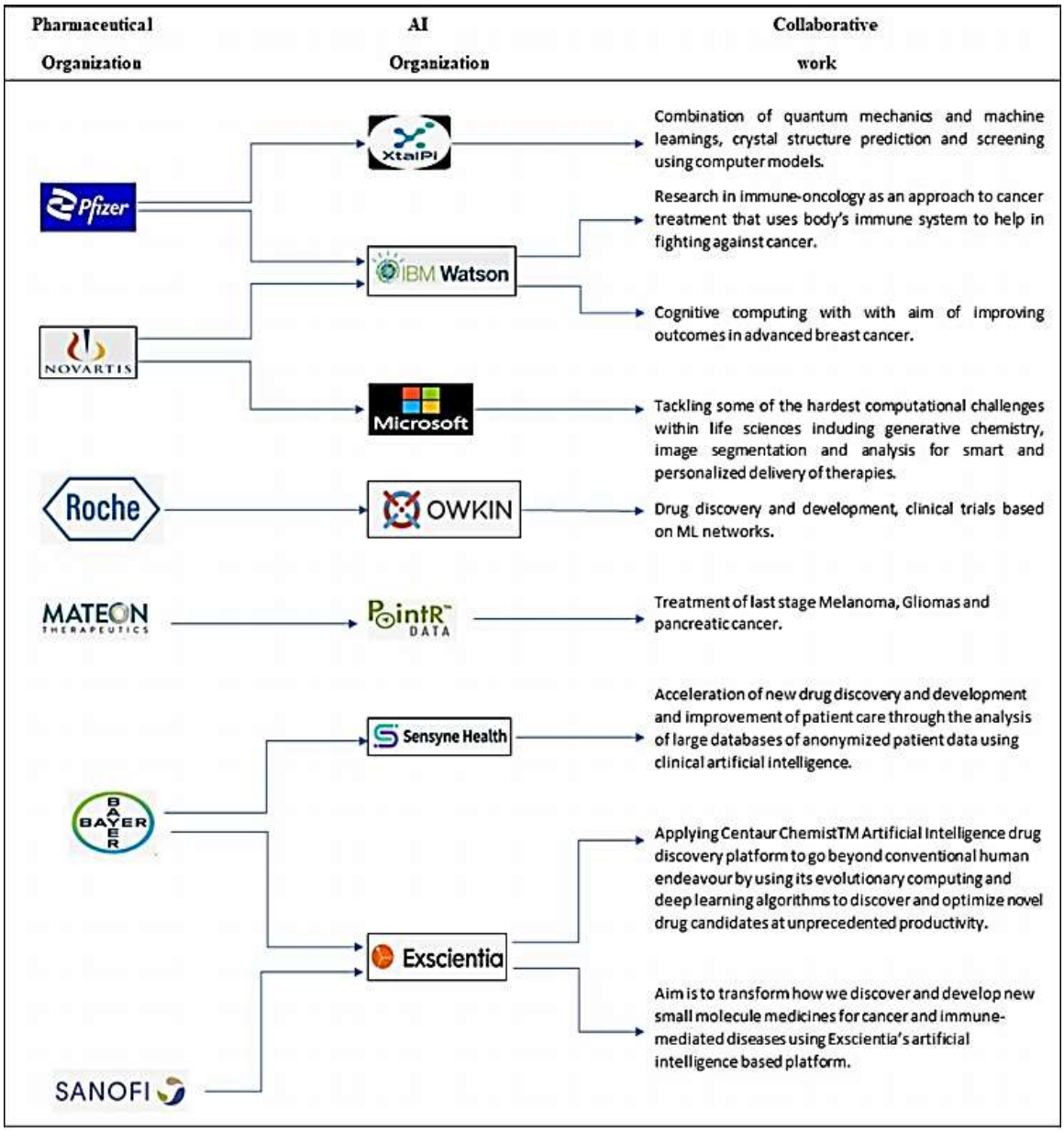

Figure 1. Leading pharmaceutical companies and their connections to AI companies that treat cancer, heart disease, and issues with the central nervous system.

APPLICATION OF AI

Discovering New Drugs

- *Medication Design:*
  - Prediction of target protein structure.
  - Interaction between drug and protein.
- *Drug Testing:*
  - Prediction of bioactivity.
  - Study of toxicity.

QA & QC

- Recognize important process parameters.
- Direct the next cycle of manufacturing.
- Use ELN and additional methods to ensure QA.

Design and Supervision of Clinical Trials

- Enrolment and selection of subjects.
- Patient discontinuation.
- Trial observation.

AI RESTRICTIONS

Despite their benefits, AI-based models have several disadvantages, including the requirement for huge datasets, possible biases, and interpretability issues. Traditional experimental techniques should be combined with AI-based models to guarantee the efficacy and safety of medications. Some of the restrictions are highlighted below:

Lack of Transparency

AI models' intricate algorithms are sometimes referred to as "black boxes" since it might be challenging to comprehend how the model makes its predictions. This lack of transparency may make it challenging to secure regulatory approval for AI-based drug development tools since it can be challenging to demonstrate that the model is making reliable and accurate predictions [21, 22].

Restricted Data Availability

A significant amount of data is required for AI algorithms to produce reliable predictions. However, there may occasionally be insufficient data available for a particular drug or population, which could lead to skewed results or less precise predictions. For instance, there may not be much data available for rare disorders, which might make developing AI models quite challenging. Results may also be skewed if the data utilized to train AI models is not representative of the intended audience. Furthermore, the lack of data sources, such longitudinal data or empirical evidence, may restrict the use of AI models. These limitations highlight how crucial it is to thoroughly assess the representatives and caliber of the data used to build AI models.

Lack of Clinical Expertise

Although AI is capable of detecting relationships, it is crucial to understand that therapies for some patients may differ despite these correlations. The statistical framework that most AI systems use may restrict their ability to understand the complex variables and the profound impacts that specific factors may have. The complex nature of treatment decisions, which are influenced by a multitude of individual factors, presents challenges for AI models that are solely focused on statistical relationships [23]. Because of this, AI might not be able to accurately capture the crucial information and implications of parameters.

Interpretation of Result

Even for subject-matter specialists, the results produced by complicated AI models might be challenging to understand. Researchers and doctors may find it difficult to comprehend and interpret the results if the models are unable to sufficiently explain how they arrived at their predictions. Converting the results into information that is helpful for clinical practice or drug research may be difficult in some circumstances. Additionally, using AI models would need a level of technical expertise that not all researchers and medical professionals can readily get, which could further limit their applicability. Therefore, it is imperative to enhance the interpretability and explainability of AI models [24, 25].

CONCLUSIONS

Final Thoughts and Prospects

All things considered, AI's role in pharmaceutical formulation and development is growing quickly and offers the sector several advantages. AI has already proven that it can evaluate vast amounts of data, accelerate clinical trials and enhance drug formulations. This has improved the precision and efficacy of the entire process while cutting down on the time and expenses associated with developing

new medications. AI has a promising future in the discovery and formulation of pharmaceuticals. It is anticipated that AI will are significantly more crucial in drug use development as it develops and advances, helping scientists find new therapeutic targets, medication relationships, and patient populations that are most likely to gain from therapy.

Additionally, when AI systems develop, they will be able to more correctly model biological systems, enabling researchers to create more individualized and potent therapies. Personalized therapy and more effective and focused medication development will follow from this. Therefore, AI's function has already proven to be innovative in pharmaceutical formulation and development, and it is anticipated to further revolutionize the industry in the next years to come. Researchers can develop more potent therapies, get new insights into complicated diseases, and enhance patient outcomes globally by utilizing AI.

REFERENCES

1. Singh D, Singh R, Gehlot A, Akram SV, Priyadarshi N, Twala B. An imperative role of digitalization in monitoring cattle health for sustainability. Electronics. 2022;11(17):2702. doi: 10.3390/electronics11172702.
2. Kalyane D, Sanap G, Paul D, Shenoy S, Anup N, Polaka S, et al. Artificial intelligence in the pharmaceutical sector: Current scene and future prospect. In: Tekade RK, editor. The Future of Pharmaceutical Product Development and Research. Academic Press; 2020. pp. 73–107. doi: 10.1016/B978-0-12-814455-8.00003-7.
3. Paul D, Sanap G, Shenoy S, Kalyane D, Kalia K, Tekade RK. Artificial intelligence in drug discovery and development. Drug Discov Today. 2021;26(1):80–93. doi: 10.1016/j.drudis.2020.10.010.
4. Landin M, Rowe RC. Artificial neural networks technology to model, understand, and optimize drug formulations. In: Formulation Tools for Pharmaceutical Development. Woodhead Publishing; 2013. pp. 7–37. doi: 10.1533/9781908818508.7.
5. Gao M, Liu S, Chen J, Gordon KC, Tian F, McGoverin CM. Potential of Raman spectroscopy in facilitating pharmaceutical formulations development–An AI perspective. Int J Pharm. 2021;597:120334. doi: 10.1016/j.ijpharm.2021.120334.
6. Sousa T, Correia J, Pereira V, Rocha M. Generative deep learning for targeted compound design. J Chem Inf Model. 2021;61(11):5343–5361. doi: 10.1021/acs.jcim.0c01496.
7. Rajalingham R, Piccato A, Jazayeri M. Recurrent neural networks with explicit representation of dynamic latent variables can mimic behavioral patterns in a physical inference task. Nat Commun. 2022;13(1):5865. doi: 10.1038/s41467-022-33581-6.
8. Huo L, Tang Y. Multi-objective deep reinforcement learning for personalized dose optimization based on multi-indicator experience replay. Appl Sci. 2023;13(1):325. doi: 10.3390/app13010325.
9. Turchin A, Masharsky S, Zitnik M. Comparison of BERT implementations for natural language processing of narrative medical documents. Informat Med Unlocked. 2023;36:101139. doi: 10.1016/j.imu.2022.101139.
10. Duch W, Swaminathan K, Meller J. Artificial intelligence approaches for rational drug design and discovery. Curr Pharm Des. 2007;13(14):1497–1508. doi: 10.2174/138161207780765954.
11. Shah H, Chavda V, Soniwala MM. Applications of bioinformatics tools in medicinal biology and biotechnology. In: Bioinformatics Tools for Pharmaceutical Drug Product Development. 2023:95–116. doi: 10.1002/9781119865728.ch6.
12. Mishra V. Artificial intelligence: The beginning of a new era in pharmacy profession. Asian J Pharm. 2018;12(2). doi: 10.22377/ajp.v12i02.2317.
13. Guo M, Kalra G, Wilson W, Peng Y, Augsburger LL. A prototype intelligent hybrid system for hard gelatin capsule formulation development. Pharm Technol. 2002 1:44–52.
14. Al Kuwaiti A, Nazer K, Al-Reedy A, Al-Shehri S, Al-Muhanna A, Subbarayalu AV, et al. A review of the role of artificial intelligence in healthcare. J Pers Med. 2023;13(6):951. doi: 10.3390/jpm13060951.

15. Hamet P, Tremblay J. Artificial intelligence in medicine. Metabolism. 2017;69:S36–S40. doi: 10.1016/j.metabol.2017.01.011.
16. Hughes JP, Rees S, Kalindjian SB, Philpott KL. Principles of early drug discovery. Br J Pharmacol. 2011;162(6):1239–1249. doi: 10.1111/j.1476-5381.2010.01127.x.
17. Mishra V. Artificial intelligence: The beginning of a new era in pharmacy profession. Asian J Pharm. 2018;12(2). doi: 10.22377/ajp.v12i02.2317.
18. Gursoy RN, Benita S. Self-emulsifying drug delivery systems (SEDDS) for improved oral delivery of lipophilic drugs. Biomed Pharmacother. 2004;58(3):173–182. doi: 10.1016/j.biopha.2004.02.001.
19. Vu GT, Phan NT, Nguyen HT, Nguyen HC, Tran YT, Pham TB, et al. Application of the artificial neural network to optimize the formulation of self-nanoemulsifying drug delivery system containing rosuvastatin. J Appl Pharm Sci. 2020;10(9):001–011. doi: 10.7324/JAPS.2020.10901.
20. Labouta HI, El-Khordagui LK, Molokhia AM, Ghaly GM. Multivariate modeling of encapsulation and release of an ionizable drug from polymer microspheres. J Pharm Sci. 2009;98(12):4603–4615. doi: 10.1002/jps.21753.
21. Kiseleva A, Kotzinos D, De Hert P. Transparency of AI in healthcare as a multilayered system of accountabilities: between legal requirements and technical limitations. Front Artif Intell. 2022;5:879603. doi: 10.3389/frai.2022.879603.
22. Kelly CJ, Karthikesalingam A, Suleyman M, Corrado G, King D. Key challenges for delivering clinical impact with artificial intelligence. BMC Med. 2019;17:1–9. doi: 10.1186/s12916-019-1426-2.
23. Davenport T, Kalakota R. The potential for artificial intelligence in healthcare. Future Healthc J. 2019;6(2):94–98. doi: 10.7861/futurehosp.6-2-94.
24. Johnson KB, Wei WQ, Weeraratne D, Frisse ME, Misulis K, Rhee K, et al. Precision medicine, AI, and the future of personalized health care. Clin Transl Sci. 2021;14(1):86–93. doi: 10.1111/cts.12884.
25. Ahmed Z, Mohamed K, Zeeshan S, Dong XQ. Artificial intelligence with multi-functional machine learning platform development for better healthcare and precision medicine. Database (Oxford). 2020;2020:baaa010. doi: 10.1093/database/baaa010.

