WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 11, 196-214. Review Article ISSN 2277–7105

ARTIFICIAL INTELLIGENCE IN HERBAL DRUG DELIVERY SYSTEMS: FORMULATION DESIGN AND OPTIMIZATION STRATEGIES

Bharat Bhushan Varma[1], Rahul Yadav[2], Rishika Yadav[3], Mukul Yadav[4]*

[1]M. Pharm Scholar, Institute of Pharmacy and Paramedical Sciences, Dr. Bhimrao Ambedkar University, Agra.

[2]Pharm. D Student, Institute of Pharmacy and Paramedical Sciences, Dr. Bhimrao Ambedkar University, Agra.

[3]B. Pharm Student, Institute of Pharmacy and Paramedical Sciences, Dr. Bhimrao Ambedkar University, Agra.

*[4]Assistant Professor, Institute of Pharmacy and Paramedical Sciences, Dr. Bhimrao Ambedkar University, Agra.

Article Received on 28 April 2026,
Article Revised on 18 May 2026,
Article Published on 01 June 2026,

https://doi.org/10.5281/zenodo.20438570

***Corresponding Author**

Mukul Yadav

M. Pharm Scholar, Institute of Pharmacy and Paramedical Sciences, Dr. Bhimrao.

How to cite this Article: Bharat Bhushan Varma[1], Rahul Yadav[2], Rishika Yadav[3], Mukul Yadav[4]*. (2026). Artificial Intelligence In Herbal Drug Delivery Systems: Formulation Design And Optimization Strategies. World Journal of Pharmaceutical Research, 15(11), 196–214.

ABSTRACT

The field of pharmaceutical sciences is undergoing a rapid transformation thanks to artificial intelligence (AI), especially in the creation of herbal drug delivery systems. Because of their natural origin, therapeutic efficacy, and fewer side effects, herbal medicines have long been used to treat and prevent a variety of disorders. However, their therapeutic use is frequently restricted by issues like poor solubility, limited bioavailability, phytoconstituent instability, and diversity in herbal composition. Advanced methods for getting around these restrictions through exact formulation design and optimization procedures have been made possible by the use of AI into herbal formulation research. Large datasets pertaining to phytochemicals, excipients, and formulation characteristics are analyzed by researchers with the aid of AI-based methods including machine learning, artificial neural networks, and predictive modeling. These methods help with regulated drug release, stability profiles of herbal formulations, nanoparticle size optimization, and drug–excipient compatibility

prediction. Additionally, AI lessens the time, expense, and experimental burden associated with traditional trial-and-error methods. Additionally, by evaluating patient-specific reactions and enhancing treatment results, AI-driven solutions facilitate customized herbal therapy. Advanced systems like liposomes, phytosomes, nanoemulsions, and polymeric nanoparticles for the targeted and prolonged release of herbal medicines have been made possible by the use of AI in herbal drug delivery. Despite a number of benefits, issues with data accessibility, regulatory acceptability, and standardization persist. All things considered, combining artificial intelligence with herbal pharmaceutics is a promising strategy for enhancing the effectiveness, safety, quality, and repeatability of herbal medications, greatly advancing drug delivery research and contemporary healthcare.

KEYWORDS: Artificial Intelligence, Machine Learning, Herbal Drug Delivery, Phytosomes, Nanoparticles, Formulation Optimization.

1. INTRODUCTION

Herbal remedies have been essential to traditional healthcare systems for ages and remain crucial in contemporary therapies.[1] Systems like Ayurveda, Unani, and Traditional Chinese Medicine actively employ phytotherapeutics owing to their therapeutic effectiveness, safety, and comprehensive disease treatment approach. Herbal formulations are commonly favored due to their association with reduced side effects, enhanced patient adherence, and prolonged safety relative to synthetic medications.[2] The rising global demand for natural and plant-based products has intensified research into herbal remedies and their pharmaceutical uses.

Notwithstanding their benefits, herbal medications encounter numerous obstacles that restrict their clinical efficacy. A significant constraint is inadequate bioavailability, resulting from low water solubility, substantial molecular size, and poor permeability of numerous phytoconstituents.[3] Moreover, herbal chemicals frequently demonstrate instability when subjected to environmental factors including light, heat, and oxygen, resulting in deterioration and diminished medicinal efficacy. A notable problem is the inconsistency in the chemical composition of herbal extracts, influenced by factors including plant source, geographical location, harvesting conditions, and extraction techniques.[4] This diversity hinders the standardization and repeatability of herbal compositions. Traditional formulation methods in pharmaceutics predominantly depend on empirical techniques and trial-and-error experimentation. These approaches necessitate considerable laboratory work, resource utilization, and extended development periods. Furthermore, conventional methods

frequently do not effectively forecast the intricate interactions among various formulation variables, particularly with herbal medications that encompass a wide array of bioactive ingredients.[5] Consequently, there is an increasing demand for sophisticated technologies that can optimize formulation development and improve the efficacy of herbal drug delivery systems.

Recent years have witnessed substantial progress in the creation of innovative drug delivery systems (NDDS) to address the limitations of natural medications. This encompasses nanoparticles, liposomes, phytosomes, nanoemulsions, and hydrogels, which are engineered to enhance solubility, stability, targeted distribution, and controlled release of active ingredients. These systems not only augment the therapeutic effetiveness of herbal medications but also decrease dose frequency and mitigate negative effects. The design and optimization of these sophisticated delivery systems entail numerous variables and intricate interactions, rendering the task arduous and time-consuming.

Artificial Intelligence (AI) has emerged as a transformative instrument in pharmaceutical research, providing novel solutions to these difficulties.[6] Artificial Intelligence denotes the emulation of human cognitive functions by machines, allowing them to acquire knowledge from data, identify patterns, and render informed decisions. In pharmaceutics, AI enables data-driven modeling, prediction, and optimization, hence diminishing dependence on traditional experimental techniques.[7] The incorporation of AI in pharmaceutical sciences has created new opportunities for expediting medication development, refining formulation precision, and augmenting overall efficiency.

A primary advantage of AI is its capacity to evaluate extensive and intricate datasets, which is especially advantageous in herbal medication development. Herbal formulations comprise numerous components and factors, complicating the establishment of obvious correlations by conventional approaches. Artificial intelligence methodologies, like machine learning and deep learning, may discern latent patterns and correlations within data, facilitating precise predictions of formulation behavior. This feature markedly diminishes the necessity for long experimental trials and facilitates the swift discovery of appropriate formulation conditions.

Artificial intelligence is essential in formulation design and optimization by forecasting physicochemical parameters, including solubility, stability, and permeability of herbal pharmaceuticals.[8] It aids in the identification of appropriate excipients by assessing

compatibility and interaction profiles. Moreover, AI models may replicate diverse formulation situations and optimize variables like as medication concentration, particle size, and release properties. This not only expedites the development process but also enhances the quality and reproducibility of the final product.

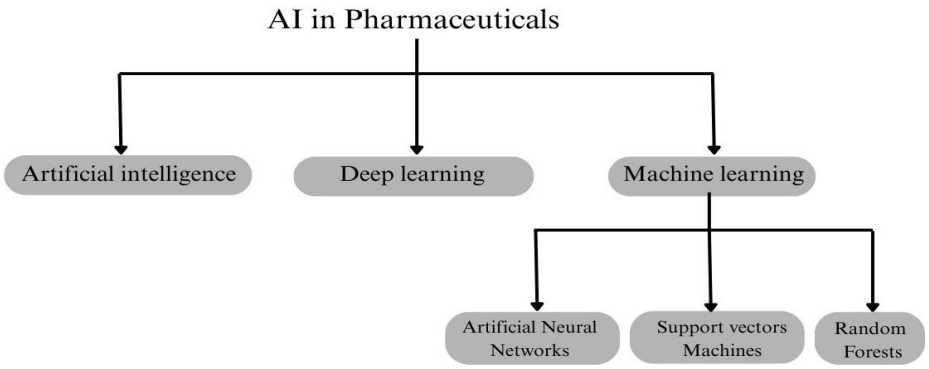
Artificial intelligence has demonstrated potential applications in the development of sophisticated carriers, including nanoparticles, liposomes, and hydrogels, inside herbal drug delivery systems.[9] These systems necessitate meticulous regulation of formulation factors to attain intended therapeutic results. AI-driven models may effectively tune these variables, guaranteeing improved drug delivery efficacy. For example, in nanoparticle formulations, AI can forecast the ideal particle size and drug loading capacity, but in gel formulations, it can enhance viscosity, spreadability, and drug release profile. Furthermore, AI enables the juxtaposition and amalgamation of conventional optimization methods, such as Design of Experiments (DoE), with sophisticated prediction models.[8] While Design of Experiments (DoE) offers a systematic methodology for experimentation, artificial intelligence (AI) provides dynamic and adaptive modeling capabilities that facilitate ongoing learning and enhancement. The integration of these methodologies strengthens the resilience and dependability of formulation development. Notwithstanding its myriad benefits, the utilization of AI in herbal pharmaceutics remains nascent and encounters specific obstacles. These factors encompass restricted access to high-quality data, the intricacy of herbal formulations, and the necessity for model validation and regulatory approval. Nonetheless, continuous research and technical progress are anticipated to mitigate these constraints and broaden the application of AI in this domain.

The incorporation of Artificial Intelligence in herbal medicine delivery systems signifies a notable progression in pharmaceutical sciences.[10] AI can enhance the formulation design, ensure precise predictions, and facilitate swift optimization, thereby addressing the issues related to herbal medications and augmenting their therapeutic efficacy. This review seeks to examine the diverse uses of AI in herbal medicine delivery systems, concentrating on formulation design and optimization methodologies, while also addressing present obstacles and future outlooks.

2. OVERVIEW OF ARTIFICIAL INTELLIGENCE IN PHARMACEUTICS

In pharmaceutics, AI is employed to model drug behavior, forecast physicochemical qualities, optimize formulations, and improve drug delivery systems.

TYPES OF AI USED IN PHARMACEUTICALS



The incorporation of AI techniques enables researchers to model various formulation situations, ascertain optimal settings, and expedite the development process. In herbal medication delivery, where diversity in phytoconstituents presents considerable problems, AI offers a systematic and reproducible method for formulation development.[11]

2.1 Artificial Intelligence (AI)

Artificial Intelligence (AI) denotes the ability of computer systems to execute tasks that usually necessitate human intelligence, including learning, reasoning, pattern recognition, and decision-making. In pharmaceutical sciences, artificial intelligence has become a revolutionary tool that enables data-driven methodologies in drug development, formulation design, and process optimization. Conventional pharmaceutical research frequently depends on empirical and trial-and-error approaches, which are laborious and resource-demanding. AI eases these constraints by facilitating the analysis of extensive and intricate datasets, hence enhancing predictive accuracy and diminishing experimental burden.[12]

2.2 Machine Learning (ML)

Machine Learning (ML), a branch of AI, employs methods that allow computers to learn from data and enhance their performance autonomously, without explicit programming. Machine learning is essential in pharmaceutical formulation since it discerns patterns and correlations between formulation variables and their responses. It facilitates predictive modeling, crucial for enhancing medication delivery systems.[13]

Several ML techniques are widely applied in pharmaceutics:

a) Artificial Neural Networks (ANN): ANN emulates the architecture and functionality of the human brain, proving especially effective in modeling nonlinear correlations between formulation variables and outcomes, such as medication release and stability. Artificial

Neural Networks (ANN) have been widely employed to forecast the efficacy of intricate formulations such as herbal nanoparticles and gels.[14]

b) Support Vector Machines (SVM): SVM is a supervised learning method employed for classification and regression tasks. It is proficient in managing high-dimensional data and is frequently utilized in forecasting drug-excipient compatibility and classifying formulation results.[8]

c) Random Forest (RF): Random Forest is an ensemble learning technique that generates several decision trees to enhance predictive accuracy. It is extensively utilized for variable selection, feature importance assessment, and prediction of formulation efficacy.[15]

Machine learning approaches substantially diminish reliance on expensive laboratory experiments by delivering precise predictions derived from existing data. This is especially advantageous in herbal drug delivery systems, where various factors affect formulation performance.

2.3 Deep Learning (DL)

Deep Learning (DL) is a sophisticated type of machine learning that use artificial neural networks with numerous hidden layers to examine intricate and high-dimensional data.[16] In contrast to conventional machine learning algorithms, deep learning can autonomously extract features from unprocessed data, rendering it exceptionally appropriate for managing intricate pharmaceutical datasets. In pharmaceutics, DL is utilized for sophisticated predictive modeling, image analysis, and simulation of drug delivery systems.[17] For example, deep learning models can forecast drug release profiles, assess stability under various settings, and analyze interactions between herbal constituents and excipients. Deep learning's capacity to analyze extensive datasets with remarkable precision renders it an invaluable asset in contemporary pharmacological research.[18]

In herbal medicine delivery, DL is especially advantageous owing to the intricacy and variety of phytochemical substances. It facilitates enhanced comprehension and forecasting of formulation behavior, therefore augmenting the efficiency and dependability of medication delivery systems.

3. HERBAL DRUG DELIVERY SYSTEMS

Herbal medications have garnered considerable interest owing to their medicinal effectiveness and diminished adverse effects. Nonetheless, their clinical utilization is frequently constrained by inadequate solubility, diminished bioavailability, instability, and fast degradation of active components.[19] Advanced drug delivery systems have been created to improve the stability, absorption, and targeted distribution of herbal medications in order to address these issues.

3.1 Nanoparticles

Nanoparticles are colloidal carriers with dimensions generally between 1 and 1000 nm. They are extensively utilized in herbal medication delivery to enhance the solubility, stability, and bioavailability of phytoconstituents.[20] Nanoparticles facilitate regulated and prolonged drug release, safeguard active chemicals against degradation, and permit targeted delivery to specific tissues. In herbal formulations, nanoparticles are especially advantageous for substances with low solubility, such as flavonoids and terpenoids. Nanoparticles boost dissolution rate and absorption by reducing particle size and increasing surface area, hence improving therapeutic efficacy.[21]

3.2 Liposomes

Liposomes are spherical vesicles formed from phospholipid bilayers capable of encapsulating both hydrophilic and lipophilic pharmaceuticals. They possess biocompatibility and biodegradability, rendering them appropriate for herbal medication delivery. Liposomes safeguard herbal components from degradation, augment medicinal stability, and raise bioavailability. They additionally provide precise delivery and regulated release. In herbal medicine, liposomes have been utilized to provide substances like curcumin and essential oils, enhancing their therapeutic efficacy.[22]

3.3 Phytosomes

Phytosomes are sophisticated herbal delivery systems that combine

TYPES OF HERBAL DRUG DELIVERY SYSTEM

Table No. 1: Herbal drug delivery systems.

System	Description	Advantages	Examples
Nanoparticles	Nano-sized carriers for herbal drugs	Improve solubility, stability, and bioavailability	Flavonoids, terpenoids
Liposomes	Phospholipid vesicles for	Controlled release and	Curcumin,

	drug encapsulation	targeted delivery	essential oils
Phytosomes	Phytoconstituent-phospholipid complexes	Enhance absorption and bioavailability	Polyphenols, herbal extracts
Herbal Gels	Semi-solid topical herbal formulations	Easy application and controlled release	Spearmint oil gel

phytoconstituents with phospholipids to improve their absorption and bioavailability. In contrast to traditional herbal extracts, phytosomes enhance the lipid solubility of active chemicals, facilitating superior contact with biological membranes.

Phytosomes have been extensively utilized for substances like flavonoids, polyphenols, and herbal extracts. They markedly augment the pharmacokinetic characteristics of herbal medications and boost therapeutic results.[23]

3.4 Herbal Gels

Herbal gels are semi-solid preparations utilized for transdermal medication administration. They provide numerous benefits, such as ease of application, non-greasy characteristics, and improved patient adherence. Herbal gels are notably efficacious for administering essential oils and botanical extracts in dermatological contexts.

For instance, spearmint oil-infused herbal gels demonstrate antimicrobial properties and enhanced skin absorption. The integration of herbal actives into gel formulations improves their stability and facilitates regulated release, rendering them effective for the treatment of skin infections and inflammation.[24]

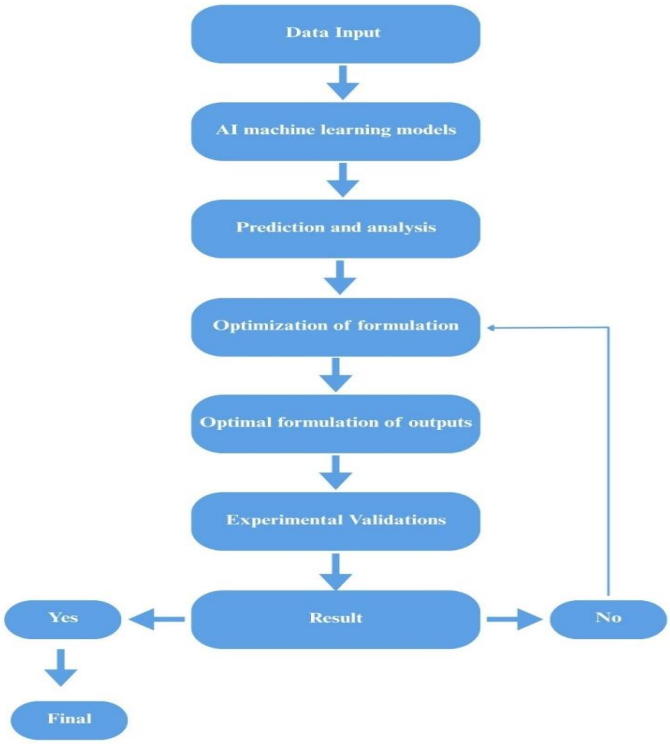
4. ROLE OF AI IN FORMULATION DESIGN

Artificial Intelligence is crucial in the design and development of pharmaceutical formulations by facilitating data-driven decision-making.[25] In conventional formulation development, numerous trials are performed to optimize variables like medication concentration, excipient ratio, and processing conditions. AI reduces the trial-and-error method by forecasting ideal formulation parameters derived from existing data.[26] Artificial intelligence methodologies are employed to forecast physicochemical characteristics, including solubility, stability, and permeability of herbal pharmaceuticals.[27] They aid in the selection of appropriate excipients by evaluating compatibility and interaction data. Moreover, AI models can enhance formulation composition by assessing the impact of various variables on formulation efficacy.

Machine learning algorithms, including Artificial Neural Networks and Random Forest, may examine extensive information and discern intricate correlations between formulation variables and responses.[28]

This allows researchers to create efficient and resilient formulations with diminished experimental effort. In herbal medication delivery, the variety of plant extracts presents obstacles, and AI offers a systematic methodology for formulation creation.[29]

PROCESS OF AI UTILIZATION IN PHARMACEUTICALS



5. AI IN OPTIMIZATION OF HERBAL FORMULATIONS

Optimization is an essential phase in pharmaceutical formulation to attain desirable attributes such as medication release, stability, and bioavailability.[30] Artificial intelligence methodologies provide sophisticated instruments for the precise and efficient optimization of formulation parameters.

AI-driven optimization entails forecasting formulation results based on input variables, facilitating the swift determination of ideal circumstances.[31] Methods such as response surface modeling and machine learning algorithms are employed to assess the impact of numerous variables concurrently.

In contrast to conventional Design of Experiments (DoE), artificial intelligence offers expedited and more precise optimization. Whereas Design of Experiments mandates predetermined experimental frameworks, artificial intelligence models can assimilate data and progressively enhance their predictive accuracy. AI is especially advantageous in intricate systems like herbal formulations, where numerous aspects affect efficacy.[32]

AI-driven optimization not only diminishes time and expense but also improves formulation quality and consistency. It facilitates the creation of resilient and effective herbal medication delivery systems that enhance therapeutic results.[33]

6. APPLICATIONS OF AI IN HERBAL DRUG DELIVERY SYSTEMS

Artificial Intelligence has been widely utilized in the advancement and enhancement of herbal medicine delivery systems. Herbal formulations comprise several bioactive substances with diverse physicochemical characteristics, rendering formulation development exceedingly intricate. Artificial intelligence methodologies offer effective computational strategies for examining these complications and enhancing formulation efficacy.

6.1 Prediction of Physicochemical Characteristics

AI algorithms can predict significant physicochemical features of herbal medications, including solubility, permeability, stability, and dissolution behavior.[34] Machine learning techniques examine experimental data to discern correlations between molecule structure and formulation efficacy. This prediction power assists researchers in choosing appropriate formulation strategies without the need for significant laboratory experimentation.

AI-driven models can assess the water solubility of phytoconstituents and forecast their stability across various environmental conditions. Such predictions are valuable for creating stable and effective herbal compositions with enhanced medicinal efficacy.[35]

6.2 Selection of Excipients and Compatibility Assessment

The selection of suitable excipients is a crucial phase in formulation development. Herbal substances may interact with excipients, resulting in instability or diminished medication release. Artificial intelligence aids in assessing drug-excipient compatibility through the analysis of physicochemical and molecular interaction data.[36]

Machine learning models can forecast compatibility between herbal actives and polymers, surfactants, or stabilizers employed in improved medication delivery systems. This diminishes formulation failures and enhances product stability and reproducibility.

6.3 Optimization of Nanoparticle Formulations

Herbal formulations utilizing nanoparticles encompass various factors, including particle size, zeta potential, drug loading, and entrapment efficiency. AI models effectively enhance these characteristics by examining formulation datasets and forecasting ideal processing conditions.

Artificial Neural Networks and Random Forest techniques are frequently employed to enhance herbal nanoparticles.[37] These models facilitate the attainment of optimal particle size distribution, regulated medication release, and improved bioavailability. AI-driven optimization minimizes experimental trials and decreases development time.[38]

6.4 Regulated and Specific Drug Administration

Artificial intelligence plays a crucial role in the advancement of regulated and precise herbal medicine delivery systems. Predictive models assist in ascertaining the impact of formulation variables on medication release kinetics and targeting efficacy.

AI can enhance polymer concentration and cross-linking density in hydrogels to facilitate the prolonged release of herbal medications.[39] Likewise, AI-enhanced targeting methodologies optimize site-specific distribution of phytoconstituents, hence improving therapeutic efficacy and minimizing systemic side effects.

6.5 Optimization of Manufacturing Processes

The production of herbal formulations entails intricate processes necessitating meticulous regulation of factors including temperature, mixing velocity, drying parameters, and pH levels.[40] Artificial intelligence facilitates real-time surveillance and enhancement of manufacturing processes via data analysis and predictive control systems. AI-driven automation promotes process uniformity, diminishes batch-to-batch variability, and elevates product quality.[41] It additionally endorses Quality by Design (QbD) methodologies in pharmaceutical production.

7. ADVANTAGES OF ARTIFICIAL INTELLIGENCE IN HERBAL PHARMACEUTICS

Artificial intelligence and computer-assisted methods have substantially enhanced herbal formulation creation by decreasing the time needed for design and alleviating experimental burdens. These tools augment predictive precision and enhance the reproducibility of formulations using data-driven optimization methodologies. They facilitate the effective optimization of intricate formulation variables and enhance the comprehension of formulation behavior and drug-excipient interactions. AI-based technologies enhance the stability, bioavailability, and therapeutic efficacy of herbal drug delivery systems. Moreover, these methodologies facilitate the formulation of individualized herbal treatments tailored to the specific requirements of patients. Advanced computational techniques enhance quality control procedures and augment manufacturing efficiency, resulting in the creation of safer, more effective, and standardized herbal compositions.[42]

AI-based approaches are especially valuable in herbal medicine due to the complexity and variability associated with plant-derived compounds.[41]

8. LIMITATIONS AND CHALLENGES OF AI IN HERBAL DRUG DELIVERY

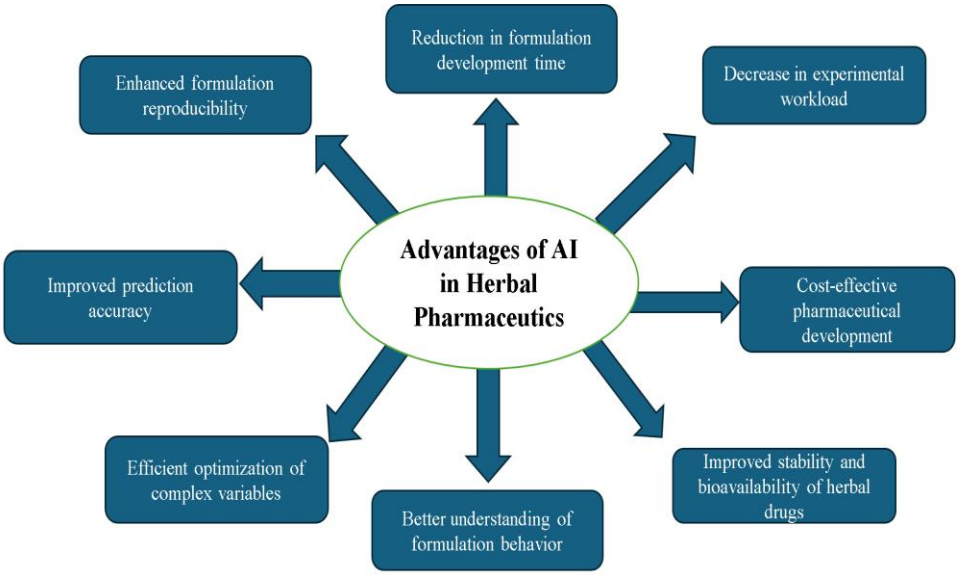
Despite its numerous advantages, AI faces several limitations in herbal pharmaceutics.

8.1 Limited Availability of Quality Data

AI models necessitate extensive and dependable datasets for precise prediction. In herbal medicine research, the availability of standardized and high-quality datasets is sometimes constrained by diversity in plant materials and extraction techniques.

8.2 Complexity of Herbal Formulations

Herbal formulations comprise many phytoconstituents exhibiting distinct.



ADVANTAGES OF AI IN HERBAL PHARMACEUTICS

chemical structures and biological activity.[42] This intricacy renders data interpretation and predictive modeling arduous.

8.3 Regulatory challenges

The application of AI in pharmaceutical formulation necessitates validation and regulatory approval. Regulatory frameworks for AI-driven pharmaceutical systems are presently in a state of evolution.[43]

Requirement for Technical Proficiency

The implementation of AI technology necessitates interdisciplinary expertise in pharmaceutics, computer science, data analytics, and programming. Insufficient expertise may hinder broad adoption.[44]

8.5 Higher Computational cost

Advanced AI and deep learning models frequently necessitate robust computer infrastructure and substantial processing capabilities, potentially elevating operational expenses.[45]

9. FUTURE PROSPECTIVES

The prospects for AI in herbal medication delivery systems are exceptionally intriguing. Ongoing progress in computer sciences, machine learning algorithms, and pharmaceutical technologies is anticipated to broaden the range of AI applications in herbal pharmaceutics. Prospective avenues for research encompass:

- Creation of AI-enhanced intelligent medicine delivery systems
- Real-time surveillance and anticipatory manufacturing
- AI-enhanced individualized herbal therapy
- Integration of artificial intelligence with nanotechnology and biotechnology
- Creation of comprehensive global databases for herbal formulations.[46]
- Utilization of artificial intelligence in pharmacokinetic and pharmacodynamic modeling.[47]
- AI-assisted clinical trials and toxicity prognosis.[48]

The integration of AI with nascent technologies like the Internet of Things (IoT), robotics, and cloud computing could significantly transform herbal pharmacological research and industrial production.

10. CONCLUSION

Artificial Intelligence has emerged as a transformative tool in pharmaceutical sciences, especially in herbal medicine delivery systems. Herbal formulations have numerous problems, such as inadequate solubility, instability, diminished bioavailability, and unpredictability of phytoconstituents. AI-driven technologies, including machine learning and deep learning, offer effective solutions for formulation design, optimization, and prediction of formulation behavior.

Artificial intelligence facilitates precise prediction of physicochemical characteristics, identification of appropriate excipients, refinement of nanoparticle formulations, and improvement of controlled drug delivery systems. In contrast to traditional trial-and-error approaches, AI markedly decreases development duration, experimental burden, and formulation expenses while enhancing precision and reproducibility.

Notwithstanding obstacles including restricted datasets, regulatory issues, and computing demands, AI persists in demonstrating significant potential in herbal pharmaceutics. Anticipated developments in AI-driven technologies are projected to enhance formulation efficiency, quality control, and personalized medicine methodologies.

The integration of Artificial Intelligence with herbal drug delivery methods signifies a significant progression in contemporary pharmaceutics and offers substantial potential for the creation of safe, effective, and novel herbal formulations.

REFERENCES

1. Balkrishna, A., Sharma, N., Srivastava, D., Kukreti, A., Srivastava, S., & Arya, V. (2024). Exploring the safety, efficacy, and bioactivity of herbal medicines: bridging traditional wisdom and modern science in healthcare. *Future Integrative Medicine*, *3*(1): 35-49.
2. Mensah, M. L., Komlaga, G., Forkuo, A. D., Firempong, C., Anning, A. K., & Dickson, R. A. (2019). Toxicity and safety implications of herbal medicines. *Herbal medicine*, *63*: 1-17.
3. Bilia, A. R., Piazzini, V., Risaliti, L., Vanti, G., Casamonti, M., Wang, M., & Bergonzi, M. C. (2019). Nanocarriers: a successful tool to increase solubility, stability and optimise bioefficacy of natural constituents. *Current medicinal chemistry*, *26*(24): 4631-4656.
4. Sun, S., Yu, Y., Jo, Y., Han, J. H., Xue, Y., Cho, M., ... & Zhuang, S. (2025). Impact of extraction techniques on phytochemical composition and bioactivity of natural product mixtures. *Frontiers in pharmacology*, *16:* 1615338.
5. Latif, R., & Nawaz, T. (2025). Medicinal plants and human health: A comprehensive review of bioactive compounds, therapeutic effects, and applications. *Phytochemistry Reviews*, 1-44.
6. Bhabad, S., Lamkhade, D., Koyate, S., Karanjkhele, K., Kale, V., & Doke, R. (2023). Transformative trends: A comprehensive review on role of artificial intelligence in healthcare and pharmaceutical research. *IP Int J Comprehensive Adv Pharmacol*, *8:* 210-9.
7. Lin, Y., Tang, J., Guo, J., Wu, S., & Li, Z. (2025). Advancing AI-enabled techniques in energy system modeling: a review of data-driven, mechanism-driven, and hybrid modeling approaches. *Energies*, *18*(4): 845.
8. Yadav, A. P., Singh, G., Singh, M. K., & Chaudhary, A. (2025). Artificial intelligence in optimizing formulations and excipients: Revolutionizing pharmaceutical product development. *Journal of Advanced Scientific Research*, *16*(07): 9-18.
9. Panchpuri, M., Painuli, R., & Kumar, C. (2025). Artificial intelligence in smart drug delivery systems: A step toward personalized medicine. *RSC pharmaceutics*, *2*(5): 882-914.
10. Patil, J., Patil, H., Panpatil, A., Chordiya, H., Deore, R., & Sanskruti, S. (2024). Advancements and challenges in the integration of artificial intelligence with herbal medicine research. *International Journal of Pharmaceutical Sciences*, *2*(4): 973-84.

11. Dangeti, A., Bynagari, D. G., & Vydani, K. (2023). Revolutionizing drug formulation: Harnessing artificial intelligence and machine learning for enhanced stability, formulation optimization, and accelerated development. *Int J Pharm Sci Med.*, *8*(8): 18.
12. Kaur, R., Kumar, R., & Aggarwal, H. (2025). Systematic Review of Artificial Intelligence, Machine Learning, and Deep Learning in Machining Operations: Advancements, Challenges, and Future Directions: R. Kaur et al. *Archives of Computational Methods in Engineering*, *32*(8): 4983-5036.
13. Dey, H., Arya, N., Mathur, H., Chatterjee, N., & Jadon, R. (2024). Exploring the role of artificial intelligence and machine learning in pharmaceutical formulation design. *International Journal of Newgen Research in Pharmacy & Healthcare*, 30-41.
14. Sowndarya, D., & Vigneshwaran, L. V. (2025). ARTIFICIAL INTELLIGENCE IN HERBAL NANO FORMULATION: A COMPREHENSIVE REVIEW. *World Journal of Applied Medical Sciences*, *2*(12): 6-13.
15. Bannigan, P., Aldeghi, M., Bao, Z., Häse, F., Aspuru-Guzik, A., & Allen, C. (2021). Machine learning directed drug formulation development. *Advanced Drug Delivery Reviews*, *175:* 113806.
16. Sarker, I. H. (2021). Deep learning: a comprehensive overview on techniques, taxonomy, applications and research directions. *SN computer science*, *2*(6): 1-20.
17. 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*(7): 1916.
18. Bhatia, N., Khan, M. M. U., & Arora, S. (2024). The role of artificial intelligence in revolutionizing pharmacological research. *Current Pharmacology Reports*, *10*(6): 323-329.
19. Ali, K. A., Mohin, S. K., Mondal, P., Goswami, S., Ghosh, S., & Choudhuri, S. (2024). Influence of artificial intelligence in modern pharmaceutical formulation and drug development. *Future Journal of Pharmaceutical Sciences*, *10*(1): 53.
20. Devi, V. K., Jain, N., & Valli, K. S. (2010). Importance of novel drug delivery systems in herbal medicines. *Pharmacognosy reviews*, *4*(7): 27.
21. Chenthamara, D., Subramaniam, S., Ramakrishnan, S. G., Krishnaswamy, S., Essa, M. M., Lin, F. H., & Qoronfleh, M. W. (2019). Therapeutic efficacy of nanoparticles and routes of administration. *Biomaterials research*, *23*(1): 20.
22. Sherry, M., Charcosset, C., Fessi, H., & Greige-Gerges, H. (2013). Essential oils encapsulated in liposomes: a review. *Journal of liposome research*, *23*(4): 268-275.

23. Barani, M., Sangiovanni, E., Angarano, M., Rajizadeh, M. A., Mehrabani, M., Piazza, S., ... & Nematollahi, M. H. (2021). Phytosomes as innovative delivery systems for phytochemicals: A comprehensive review of literature. *International journal of nanomedicine*, 6983-7022.
24. Hao, H., Zheng, X., & Wang, G. (2014). Insights into drug discovery from natural medicines using reverse pharmacokinetics. *Trends in pharmacological sciences*, *35*(4): 168-177.
25. Yang, B., Xu, J., Liu, S., Wu, C., Li, Y., Lv, M., ... & Wang, G. (2025). Applications of bioactive herbal extracts in dressing materials for skin wound repair: Ingredients, mechanisms and innovations. *Interdisciplinary Medicine*, *3*(4): e20240117.
26. Schwartz, J. B., O'Connor, R. E., & Schnaare, R. L. (2002). Optimization techniques in pharmaceutical formulation and processing. In *Modern pharmaceutics* (pp. 921-950). CRC Press.
27. Ali, K. A., Mohin, S. K., Mondal, P., Goswami, S., Ghosh, S., & Choudhuri, S. (2024). Influence of artificial intelligence in modern pharmaceutical formulation and drug development. *Future Journal of Pharmaceutical Sciences*, *10*(1): 53.
28. Aungst, B. J. (2017). Optimizing oral bioavailability in drug discovery: an overview of design and testing strategies and formulation options. *Journal of pharmaceutical sciences*, *106*(4): 921-929.
29. Lauro, C. H., Pereira, R. B., Brandão, L. C., & Davim, J. P. (2015). Design of Experiments—Statistical and artificial intelligence analysis for the improvement of machining processes: A review. *Design of experiments in production engineering*, 89-107.
30. Okuyelu, O., & Adaji, O. (2024). AI-driven real-time quality monitoring and process optimization for enhanced manufacturing performance. *J. Adv. Math. Comput. Sci.*, *39*(4): 81-89.
31. Ola, M., Bhaskar, R., Patil, P. S., Badgujar, S. V., & Haswani, N. G. (2025). Formulation and Delivery Issues for Active Ingredients of Herbal Medicines, Nutraceuticals, and Cosmetics: Comparisons to Small-Molecule Drugs. *Formulating Pharma-, Nutra-, and Cosmeceutical Products from Herbal Substances: Dosage Forms and Delivery Systems*, 163-191.
32. Bannigan, P., Aldeghi, M., Bao, Z., Häse, F., Aspuru-Guzik, A., & Allen, C. (2021). Machine learning directed drug formulation development. *Advanced Drug Delivery Reviews*, *175:* 113806.

33. Tripathi, G. AI-driven predictive modeling for enhancing drug solubility and stability in pharmaceutical formulations.
34. Omari, D. M., Akkam, Y., & Sallam, A. (2021). Drug-excipient interactions: an overview on mechanisms and effects on drug stability and bioavailability. *Annals of the Romanian Society for Cell Biology*, *25*(4): 8402-8429.
35. Rathore, N., & Rajan, R. S. (2008). Current perspectives on stability of protein drug products during formulation, fill and finish operations. *Biotechnology progress*, *24*(3): 504-514.
36. Bulut, S., Aasim, M., Emsen, B., Ali, S. A., Askin, H., & Karatas, M. (2025). Machine learning modeling and response surface methodology driven antioxidant and anticancer activities of chitosan nanoparticle-mediated extracts of Bacopa monnieri. *International Journal of Biological Macromolecules*, *310*: 143470.
37. Tekade, R. K., & Saraf, S. (Eds.). (2026). *Biomolecular and Safety Considerations of Phytopharmaceuticals*. CRC Press.
38. Nithyanantham, D., Nair, A., & Nayak, U. Y. (2025). Leveraging artificial intelligence for advancements in liquid dosage formulations in the pharmaceutical industry. *Therapeutic Innovation & Regulatory Science*, *59*(5): 1004-1031.
39. Kumbhar, P., Pandey, N. K., Kumar, B., & Vinchurkar, K. (2024). Artificial intelligence in herbal medicine formulations. In *AI innovations in drug delivery and pharmaceutical sciences; advancing therapy through technology* (pp. 147-162). Bentham Science Publishers.
40. 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*(7): 1916.
41. Kalita, I., Bhattacharjee, S., & Saharia, M. (2025). Advancements in medicinal plant research: Harnessing artificial intelligence, machine learning, deep learning, and bioinformatics. In *Biotechnology, Multiple Omics, and Precision Breeding in Medicinal Plants* (pp. 135-145). CRC Press.
42. Wang, H., Chen, Y., Wang, L., Liu, Q., Yang, S., & Wang, C. (2023). Advancing herbal medicine: enhancing product quality and safety through robust quality control practices. *Frontiers in pharmacology*, *14:* 1265178.
43. Arunkumar, M., Rajkumar, K., Jeyaseelan, W. R., & Natraj, N. A. (2025). Data mining, machine learning, and statistical modeling for predictive analytics with behavioral big data. *Tehnički vjesnik*, *32*(1): 72-77.

44. Lenarczyk, G., Minssen, T., Price, N., & Rai, A. (2025). The future of AI regulation in drug development: a comparative analysis. *Journal of Law and the Biosciences*, *12*(2): lsaf028.
45. Rane, N. L., Paramesha, M., Choudhary, S. P., & Rane, J. (2024). Artificial intelligence, machine learning, and deep learning for advanced business strategies: a review. *Partners Universal International Innovation Journal*, *2*(3): 147-171.
46. Behgounia, F., & Zohuri, B. (2020). Artificial intelligence integration with nanotechnology. *Nano Tech Appl*, *3*(1): 1-7.
47. Chen, H., Liu, Z., Du, Y., Meng, X., Xue, L., Sun, X., ... & Wang, S. (2025). Comparative analysis of Chinese classical prescriptions and global traditional polyherbal formulations: insights from the database of global polyherbal formulation (GPFD). *Chinese Medicine*, *20*(1): 169.
48. Basile, A. O., Yahi, A., & Tatonetti, N. P. (2019). Artificial intelligence for drug toxicity and safety. *Trends in pharmacological sciences*, *40*(9): 624-635.