

REVIEW ARTICLE



A Review on Current Progress, Bottlenecks, and Future Prospects of Using Algorithmic and Computational Optimization of Drug Delivery Systems

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Abstract: Modern drug delivery paradigms increasingly depend on algorithmic computation to resolve longstanding challenges in bioavailability, target site specificity, and controlled release dynamics. Advanced artificial intelligence models, including machine learning ensembles, deep neural networks, and reinforcement learning, enable predictive modeling of critical formulation variables, nanoparticle assemblies, and pharmacokinetics. Integrations of computational models with physiologically based pharmacokinetic models facilitate precise mapping of absorption, distribution, metabolism, excretion, and toxicity profiles prior to experimental execution. The convergence of computational intelligence with bio-fabrication techniques, such as three-dimensional bioprinting, allows the precise spatial arrangement of therapeutics within bio-compatible matrices, while closed-loop systems linked to the Internet of Medical Things permit real-time dosage adjustments driven by continuous physiological inputs. Despite these advancements, significant bottlenecks impede widespread clinical translation, notably data heterogeneity, algorithmic opacity, material degradation complexities, and evolving regulatory standards for adaptive software architectures. Addressing these limitations requires robust physics-informed neural networks, standardized data repositories, and transparent explainability models to validate computational predictions against empirical biological outcomes. Algorithmic drug delivery represents a fundamental shift from empirical formulation design toward precise, patient-specific therapeutic interventions.

Keywords: Machine Learning; Smart Nanocarriers; Predictive Pharmacokinetics; Internet of Medical Things; Personalized Therapeutics.

1. Introduction

Pharmaceutical drug delivery has transformed from rudimentary immediate-release oral and parenteral forms to complex micro- and nano-structured therapeutic vector systems [1]. Historical formulations relied primarily on passive dissolution kinetics and mass transport driven by concentration gradients, which frequently yielded suboptimal bioavailability, erratic systemic exposure, and high off-target toxicity [2]. The development of liposomes, polymeric nanoparticles, micro-emulsions, and hydrogels offered initial solutions for targeted localized action and sustained release [3]. However, these traditional delivery systems remain bound by deterministic engineering paradigms that fail to account for inter-individual biological heterogeneity, dynamically changing disease states, and complex in vivo physiological barriers [4]. Achieving dynamic therapeutic responses requires systems capable of processing real-time physiological signals and modulating drug release kinetics accordingly [5].

The integration of computational data analytics into pharmaceutical sciences marks a major technological shift [6]. Artificial intelligence paradigms facilitate the interpretation of high-dimensional bio-molecular datasets, structural chemical descriptors, and physiological metrics [7]. Computational methods reduce empirical trial-and-error in pharmaceutical development, replacing resource-intensive lab evaluations with in silico screening and optimization [8]. Advanced algorithms predict molecular interactions, drug-excipient phase behavior, particle aggregation kinetics, and membrane permeability prior to wet-lab synthesis [9]. Consequently, data-driven models accelerate formulation timelines, reduce material costs, and maximize therapeutic stability [10].

Developing targeted drug delivery systems requires balancing multiple competing formulation criteria [11]. Engineers must optimize particle diameter, surface charge, encapsulation efficiency, core-shell morphology, ligand density, and degradation rates within narrow therapeutic windows [12]. Biological barriers in disease states such as the blood-brain barrier, dense tumor stroma, and mucosal clearance vectors complicate targeted delivery [13]. Traditional response surface methodologies and linear statistical models

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cannot fully capture non-linear interactions across multivariable formulation spaces [14]. Artificial intelligence models effectively navigate these complex spaces by mapping high-order non-linear interactions, identifying optimal formulation parameters, and anticipating biological responses across diverse patient populations [15].

2. Machine Learning and Computational Models in Drug Formulation

2.1. Supervised and Unsupervised Machine Learning Architectures

Supervised machine learning forms the foundation of modern computational formulation design [16]. Algorithms such as Support Vector Machines (SVM), Random Forests (RF), and Gradient Boosting Machines (GBM) classify and predict outcomes based on labeled historical datasets [17]. In formulation optimization, SVM architectures classify binary outcomes such as stable versus unstable nano-emulsions, using hyperplanes mapped across non-linear feature spaces [18]. Random Forest decision trees aggregate predictions from multiple bootstrapped samples, making them effective for handling noisy experimental data when evaluating drug loading capacity and particle size distributions [19]. The k-Nearest Neighbors (k-NN) algorithm predicts drug solubility profiles and bioavailability patterns by comparing target compound physicochemical descriptors to known molecular spaces [20]. Unsupervised learning models, including Principal Component Analysis (PCA) and k-means clustering, identify hidden patterns in chemical libraries without prior labeling, isolating favorable excipient profiles for specific drug classes [21]. A summary of core machine learning algorithms and their specific operational domains in pharmaceutical development is presented in Table 1.

Table 1. Computational performance metrics and applications of machine learning algorithms in formulation design.

Algorithm Type	Machine Learning Model	Input Descriptors	Target Pharmaceutical Application	Operational Performance Measure
Supervised	Support Vector Machines (SVM)	Molecular weight, log P, polar surface area, lipid composition	Phase stability prediction in nano-emulsions and liposomes	Classification Accuracy, AUC-ROC
Supervised	Random Forests (RF)	Polymer ratio, solvent density, homogenization speed, temperature	Particle size distribution and encapsulation efficiency optimization	Mean Squared Error (MSE), R ² coefficient
Supervised	k-Nearest Neighbors (k-NN)	Topological polar surface area, hydrogen bond counts, solubility	Oral bioavailability classification and dissolution profiling	Sensitivity and Specificity
Supervised	Gradient Boosting Machines (GBM)	Excipient ratios, viscosity, surfactant HLB values	Drug release rate modeling and stability forecasting	Root Mean Squared Error (RMSE)
Unsupervised	Principal Component Analysis (PCA)	Multi-omics parameters, structural fingerprint vectors	Dimensionality reduction of large chemical libraries	Explained Variance Ratio
Unsupervised	k-Means Clustering	Physicochemical screening metrics, lipophilicity profiles	Excipient grouping and biocompatibility stratification	Silhouette Coefficient

2.2. Deep Learning Architectures and Multi-Omics Integration

Deep learning models handle high-dimensional biological data using multi-layered hierarchical structures [22]. Convolutional Neural Networks (CNNs) extract spatial features from high-content cellular imaging and structural molecular grids [23]. Recurrent Neural Networks (RNNs) and Long Short-Term Memory (LSTM) networks process sequential time-series data, capturing continuous drug release profiles, blood concentration dynamics, and biosensor telemetry [24]. Autoencoder models reduce data dimensionality, extracting key low-dimensional features from extensive multi-omics datasets [25]. Integrating genomics, transcriptomics, proteomics, and metabolomics using deep learning models reveals individual metabolic variations, informing the tailored design of targeted delivery vectors [26].

2.3. Adaptive Control via Reinforcement Learning

Reinforcement Learning (RL) optimizes decision-making by evaluating actions against system rewards within simulated or operational environments [27]. In adaptive drug delivery, RL agents evaluate physiological feedback, such as blood glucose concentrations or inflammatory biomarker levels, to dynamically adjust therapeutic delivery [28]. The mathematical models rely on Markov Decision Processes (MDP), expressed as:

$$S_{t+1} = f(S_t, A_t)$$

where the state transition S_{t+1} depends on the current physiological state S_t and the delivered therapeutic action A_t [29]. The RL agent optimizes a cumulative reward function R_t , maximizing therapeutic efficacy while penalizing off-target toxicity [30]:

$$R_t = \sum_{k=0}^{\infty} \gamma^k r_{t+k+1}$$

where $\gamma \in [0,1)$ represents the discount factor prioritizing immediate versus long-term physiological outcomes [31]. This control loop enables self-correcting delivery systems, such as automated subcutaneous insulin pumps or localized chemotherapy implants [32].

2.4. Hybrid Physics-Informed and Explainable AI Models

Despite high predictive accuracy, purely data-driven deep learning models often operate as opaque "black boxes," limiting clinical trust and regulatory approval [33]. Physics-Informed Neural Networks (PINNs) address this challenge by embedding fundamental conservation laws, fluid dynamics, and mass-transfer equations directly into the neural network loss function [34]. Incorporating Fickian diffusion equations directly into model training ensures that predictions conform to physical transport constraints:

$$\frac{\partial C}{\partial t} = D \nabla^2 C$$

where C represents drug concentration, t denotes time, and D signifies the diffusion coefficient [35]. Concurrently, Explainable Artificial Intelligence (XAI) tools, such as SHapley Additive exPlanations (SHAP) and Local Interpretable Model-agnostic Explanations (LIME), quantify feature contributions to model predictions [36]. XAI elucidates how specific molecular weight fractions, surfactant concentrations, or polymer ratios drive predicted release kinetics, ensuring transparency for regulatory compliance and safety validation [37].

3. AI-Guided Engineering of Advanced Nanocarrier Systems

3.1. Predictive Formulation Optimization and Excipient Selection

Designing stable nanocarriers requires navigating complex multidimensional chemical spaces [18]. Machine learning models replace empirical trial-and-error by predicting optimal surfactant ratios, lipid compositions, and polymer blends [38]. Quantitative Structure-Property Relationship (QSPR) models map excipient chemical structures to key stability indicators, such as zeta potential, polydispersity index (PDI), and encapsulation efficiency [39]. Computational screening tools rapidly evaluate vast excipient databases to identify optimal stabilizer combinations, minimizing phase separation, drug leakage, and Ostwald ripening [40]. A comparison between conventional empirical strategies and computational AI-guided design methods is shown in Table 2.

Table 2. Comparison of traditional empirical methods versus AI-guided design strategies in advanced nanocarrier engineering.

Design Criteria	Traditional Empirical Methods	Computational AI-Guided Methods	Advantages
Excipient Selection	Empirical screening and manual compatibility testing	QSPR modeling and deep chemical structure screening	Rapid identification of compatible matrices, preventing phase separation
Encapsulation Optimization	Manual trial-and-error adjustments	Deep learning and neural network interaction mapping	Maximized drug payload capacity with minimal material waste
Morphological Control	Post-fabrication electron microscopy	Generative Adversarial Networks and predictive simulation	Targeted size and shape design tailored for tissue clearance vectors
Targeted Ligand Conjugation	Literature-guided affinity trials	In silico molecular docking and binding dynamics simulation	Enhanced targeting specificity, reducing off-target systemic toxicity
Release Kinetics Modeling	Empirical mathematical fitting (Higuchi, Peppas)	Physics-informed LSTM time-series networks	Precise prediction of multi-phase and non-Fickian drug release
Pre-clinical Toxicity Screening	In vitro cell assays and animal models	Quantitative Structure-Toxicity Relationship (QSTR) models	Early detection of cellular toxicity, minimizing animal usage

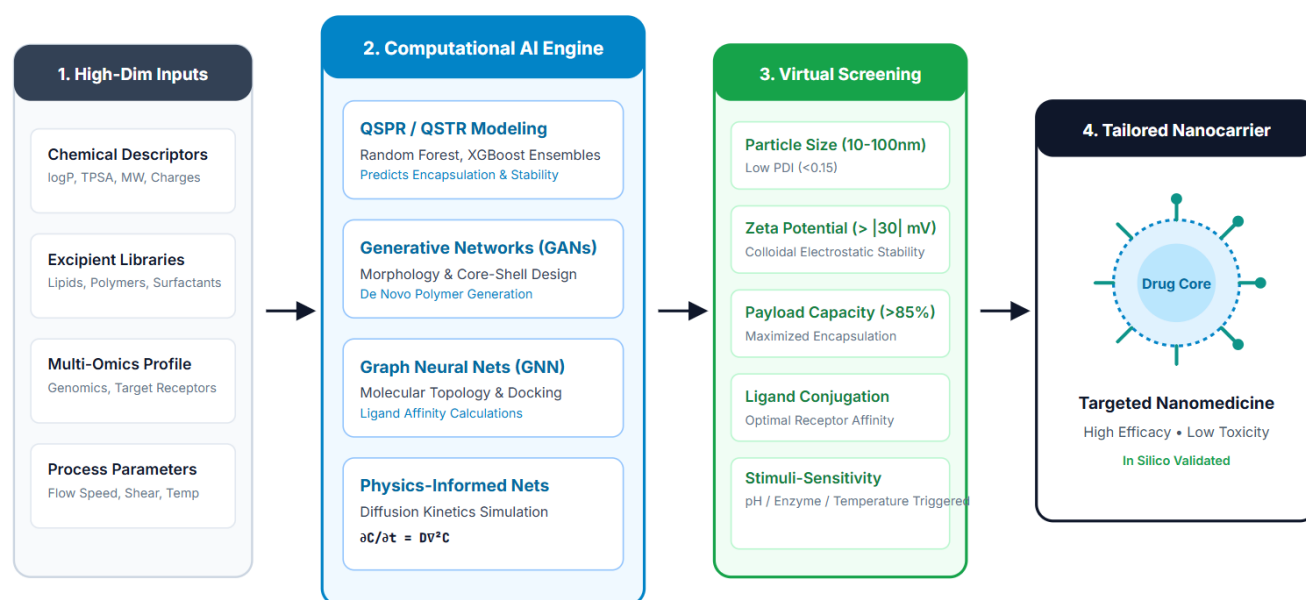


Figure 1. Multistage AI-guided computational process for preparation of nanocarrier.

3.2. Stimuli-Responsive Vector Design and Surface Functionalization

Smart nanocarriers respond to localized micro-environmental triggers, including pH gradients, redox states, enzymatic concentrations, and temperature variations [41]. Machine learning models optimize these responsive systems by predicting structural phase changes in smart polymers under specific biological conditions [42]. Surface functionalization with targeting ligands such as antibodies, peptides, or aptamers is optimized via computational docking algorithms and molecular dynamics simulations [43]. These computational tools calculate binding affinities between modified nanocarrier surfaces and target cell surface receptors, ensuring optimal spatial arrangement and ligand density to enhance receptor-mediated endocytosis [44].

3.3. Diagnostic Marker Separation versus Therapeutic Delivery Outcomes

A critical distinction must be maintained between computational models for diagnostic biomarker detection and those controlling therapeutic drug delivery [45]. Diagnostic AI models evaluate imaging signals, fluid biomarkers, or histological features to identify disease states [46]. In contrast, therapeutic AI models predict and control vector transport, drug loading efficiency, membrane permeability, release kinetics, and systemic clearance [47]. Confounding diagnostic algorithms with delivery control mechanisms can lead to errors in clinical design [48]. Diagnostic output must serve strictly as an input parameter for therapeutic decision algorithms, maintaining a clear separation between disease detection and dynamic therapeutic intervention [49].

4. Predictive Pharmacokinetics, Pharmacodynamics, and Biopharmaceutics

4.1. Computational ADMET Profiling and Molecular Property Prediction

Predicting Absorption, Distribution, Metabolism, Excretion, and Toxicity (ADMET) early in formulation development reduces late-stage clinical attrition [29]. Machine learning models process molecular descriptors such as octanol-water partition coefficients (log P), topological polar surface area (TPSA), hydrogen bond donors/acceptors, and rotatable bonds to forecast in vivo drug behavior [50]. Graph Neural Networks (GNNs) extract topological features directly from molecular structures, predicting intestinal membrane permeability, cytochrome P450 enzyme inhibition, and renal clearance rates [51]. Quantitative Structure-Toxicity Relationship (QSTR) models identify structural alerts for hepatotoxicity, cardiotoxicity (e.g., hERG channel inhibition), and immunogenicity, facilitating early modification of therapeutic vectors [52].

4.2. AI-Enhanced Physiologically Based Pharmacokinetic (PBPK) Modeling

Physiologically Based Pharmacokinetic (PBPK) models use mathematical structures to simulate drug movement through anatomical compartments linked by blood flow [31]. Using artificial intelligence in traditional PBPK models addresses parameter estimation challenges caused by physiological variability [53]. Machine learning algorithms optimize differential equations governing compartmental transport:

$$\frac{dC_i}{dt} = \frac{Q_i}{V_i} \left(C_{art} - \frac{C_i}{K_{p,i}} \right)$$

where C_i represents drug concentration in tissue i , V_i denotes tissue volume, Q_i is blood flow rate, C_{art} is arterial drug concentration, and $K_{p,i}$ is the tissue-to-plasma partition coefficient [32]. Machine learning models dynamically estimate tissue partition coefficients ($K_{p,i}$) based on compound physicochemical properties and local tissue lipid/protein compositions [54]. This hybrid model improves predictions of non-linear kinetics, carrier clearance, and drug accumulation across healthy and diseased populations [55].

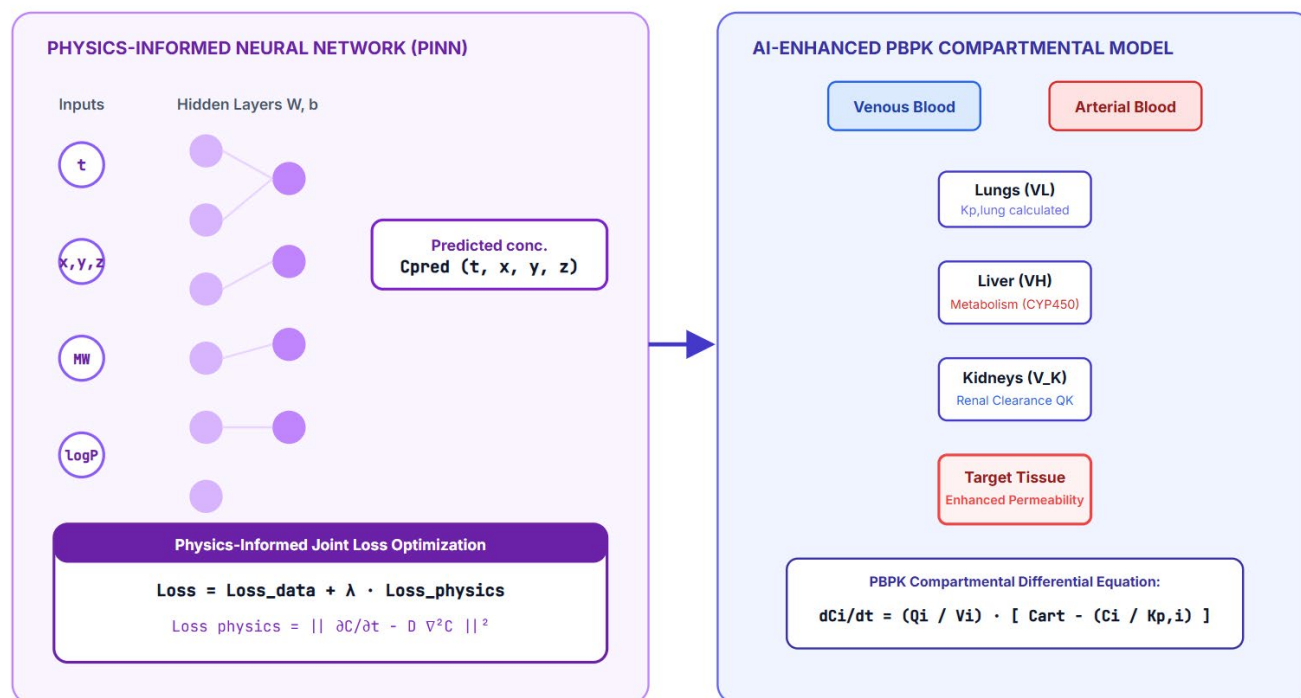


Figure 2. Process for differentiating diagnostic prediction pathways from therapeutic execution control loops in advanced drug delivery.

5. Convergence of AI with IoMT and Bio-Sensing Platforms

5.1. Real-Time Biosensing and Dynamic Physiological Data Acquisition

The integration of Artificial Intelligence with the Internet of Medical Things (IoMT) enables continuous biological data processing and dynamic therapeutic monitoring [34]. Wearable and implantable biosensors collect real-time physiological metrics, including interstitial glucose concentrations, local pH shifts, electrodermal responses, body temperature, and pulse rate [56]. Machine learning algorithms process these time-series data streams, filtering out noise and motion artifacts to extract accurate biomarker trends [57]. This telemetry forms the foundation for context-aware therapeutic platforms that adapt to dynamic physiological changes [58].

5.2. Closed-Loop Delivery Mechanisms and Autonomous Control

Closed-loop therapeutic systems unite real-time biosensing, automated data analysis, and controlled drug administration into a self-regulating control system [36]. The control system processes biological inputs, projects target physiological trajectories, and calculates necessary dosage adjustments [59].

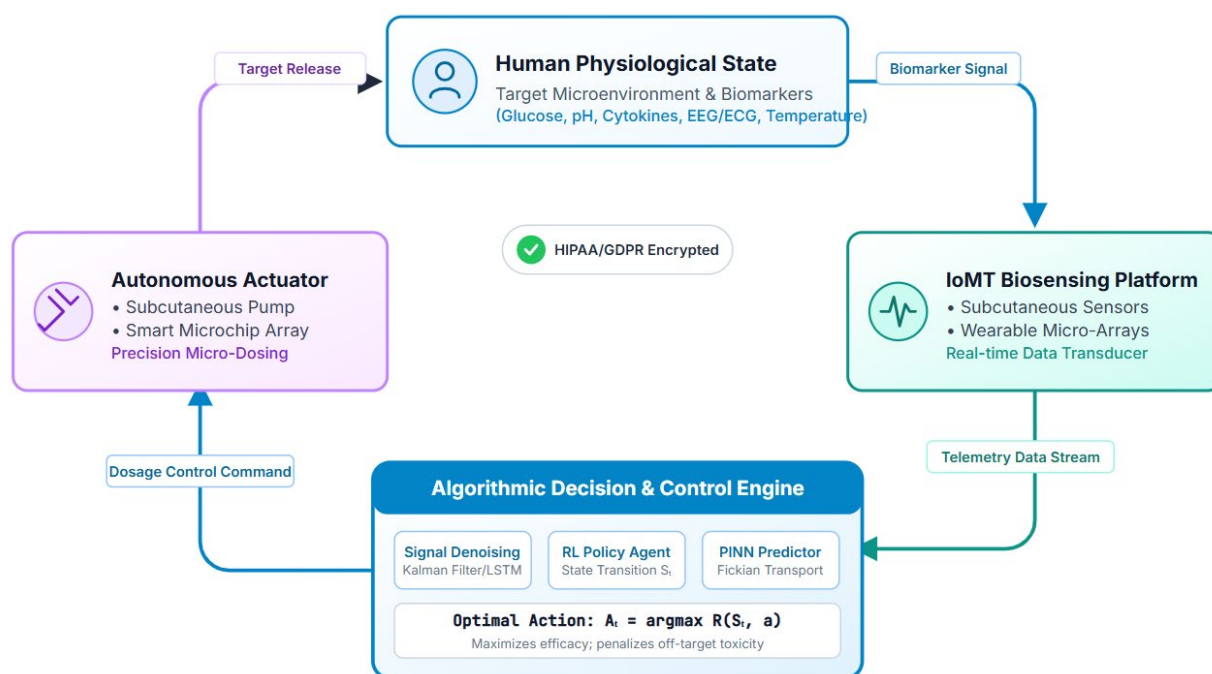


Figure 3. AI-driven closed-loop therapeutic drug delivery system operating via real-time biological feedback.

As shown in Figure 3, continuous physiological feedback is transmitted through biosensor telemetry directly to an AI controller, which computes exact release commands for the actuator.

The predictive engine processes these trends against historical patient profiles, returning modulated actuation commands to precision delivery devices.

5.3. Digital Security, Data Integrity, and Interoperability

Connecting drug delivery devices to public networks introduces critical data privacy and cybersecurity risks [43]. Unauthorized access to delivery device algorithms could alter dosage parameters, presenting severe safety hazards [61, 62]. Implementing robust cryptographic standards, end-to-end data encryption, and secure hardware architecture is essential [63]. Algorithms must process data securely in compliance with international privacy regulations, such as HIPAA and GDPR [64]. Establishing standardized interoperability protocols enables seamless, secure data exchange among sensors, delivery actuators, and electronic health records without compromising system safety [65].

6. Bioprinting, Smart Implants, and Site-Specific Delivery Devices

6.1. AI Optimization of Rheology and Structural Architecture in 3D Bioprinting

Three-dimensional bioprinting allows the precise fabrication of drug-loaded scaffolds and complex tissue constructs [55]. However, optimizing bio-ink formulations requires balancing competing rheological properties [66]. Bio-inks must exhibit shear-thinning behavior to flow smoothly during extrusion, alongside rapid structural recovery post-extrusion to maintain scaffold integrity [67]. Machine learning models analyze bio-ink compositions including hydrogel polymer densities, crosslinking agents, and drug loadings to predict viscosity, shear stress profiles, and printability [68]. Deep learning generative models optimize internal porous geometries to tune matrix degradation kinetics and drug diffusion rates [69].

6.2. Intelligent Implantable Systems and Autonomous Feedback Control

Implantable therapeutic devices offer controlled, localized, long-term drug release, overcoming compliance challenges associated with frequent dosing schedules [62]. Integrating onboard microcontrollers running lightweight AI models transforms these implants into intelligent, self-regulating delivery platforms [70]. Microchip delivery arrays can store multiple distinct therapeutic agents within micro-reservoirs, releasing specific doses in response to real-time biosensor inputs [71]. For instance, deep brain stimulation devices

coupled with micro-fluidic channels adjust local neurotransmitter delivery upon detecting electroencephalographic signatures of parkinsonian tremors or seizure activity [72].

6.3. Generative Biomaterial Discovery and Interfacial Biocompatibility

Developing long-term bio-implants requires materials that minimize foreign body responses, fibrotic encapsulation, and chronic inflammation [71]. Generative artificial intelligence architectures, such as Generative Adversarial Networks (GANs) and Variational Autoencoders (VAEs), generate novel biomaterial structures with tailored mechanical and surface properties [73]. Computational models screen surface energy, hydrophilicity, and micro-topography to minimize protein adsorption and immune cell activation [74]. AI-guided screening identifies biocompatible compositions that integrate smoothly with surrounding biological tissue while maintaining target drug release profiles [75].

7. Ethical, Regulatory, and Translational Bottlenecks

7.1. Data Heterogeneity, Bias, and Algorithmic Robustness

A primary bottleneck in deploying predictive drug delivery models is the quality and homogeneity of training data [78]. Pharmaceutical data repositories are frequently fragmented, incomplete, or collected under non-standardized experimental conditions [79]. Machine learning models trained on biased or limited demographic datasets risk poor generalization, leading to inconsistent dose predictions across diverse patient populations [80]. Addressing these imbalances requires establishing standardized, open-access databases, enforcing rigorous data curation, and deploying privacy-preserving federated learning architectures [81].

7.2. Interpretability, Algorithmic Transparency, and Regulatory Compliance

Regulatory guidelines established by authorities such as the US Food and Drug Administration (FDA) and the European Medicines Agency (EMA) require predictable, deterministic safety and efficacy profiles [81]. Deep learning models operate through complex, non-linear feature transformations that resist simple interpretation, complicating traditional regulatory review [82]. Regulatory bodies are developing guidelines for Software as a Medical Device (SaMD) and adaptive artificial intelligence applications [83]. Establishing clear validation standards, deterministic performance boundaries, and robust XAI integration is necessary to ensure safety and secure regulatory approval [84].

7.3. Equitable Access and Clinical Implementation Barriers

Advanced computational drug delivery systems carry high development and manufacturing costs, which may limit equitable global access [83]. High production costs for smart implants, bioprinted scaffolds, and IoMT infrastructure risk exacerbating healthcare disparities between high- and low-resource settings [85]. Widespread clinical adoption requires simplifying device hardware, lowering manufacturing costs, and establishing scalable manufacturing protocols [86]. Ensuring equitable distribution requires deliberate policies, open-source computational tools, and cost-effective material engineering [87].

8. Future Prospects

8.1. Quantum Machine Learning and Generative Artificial Intelligence

Quantum Computing (QC) holds immense promise for transforming computational pharmaceuticals [86]. Quantum Machine Learning (QML) uses quantum bits (qubits) to process complex molecular interactions exponentially faster than classical supercomputers [88]. QML algorithms can simulate complex quantum mechanical interactions governing drug-carrier binding, lipid membrane crossing, and multi-phase degradation kinetics with high precision [89]. Concurrently, generative AI architectures continue to refine drug carrier design, rapidly outputting novel nanocarrier formulations optimized for high drug loading and minimal toxicity [90].

8.2. Digital Twins and Real-World Evidence Integration

The concept of the "Digital Twin" a dynamically updated virtual model of a patient's physiological state is transforming personalized therapeutics [85]. Integrating continuous biosensor telemetry, multi-omics profiles, and clinical records into a computational twin enables real-time simulation of drug transport and response [91]. Researchers can evaluate multiple dosing strategies, carrier designs,

and administration schedules in silico prior to clinical delivery [92]. Combining digital twins with real-world evidence collected across diverse clinical populations will enhance therapeutic efficacy, minimize adverse events, and advance precision medicine [93].

9. Conclusion

Artificial intelligence is transforming pharmaceutical drug delivery from empirical formulation design into a precise, predictive engineering discipline. Machine learning, deep neural networks, and reinforcement learning enable optimized nanocarrier fabrication, highly accurate pharmacokinetic modeling, and dynamic, self-regulating drug delivery systems. The combination of computational intelligence with three-dimensional bioprinting and the Internet of Medical Things provides powerful tools for personalized therapeutics. Overcoming translation hurdles such as data heterogeneity, model opacity, device security, and evolving regulatory standards requires ongoing interdisciplinary collaboration among pharmaceutical scientists, computational engineers, clinicians, and regulatory authorities. Algorithmic drug delivery will play a crucial role in advancing safe, target-specific, and fully individualized therapeutic interventions as physics-informed models, explainable architectures, and digital twin platforms continue to mature

References

- [1] Aundhia C, Parmar G, Talele C, Shah N, Talele D. Impact of artificial intelligence on drug development and delivery. *Current Topics in Medicinal Chemistry*. 2024;24(3):180-195.
- [2] Ekpan FM, Ori MO, Samuel HS, Egwuatu OP. The synergy of AI and drug delivery: A revolution in healthcare. *International Journal of Advanced Biological and Biomedical Research*. 2024;12(1):45-67.
- [3] Biswas M. AI-powered nanorobots: A mini review on innovations in healthcare. *Journal of Artificial Intelligence*. 2024;1(2):1-4.
- [4] Kapoor DU, Sharma JB, Gandhi SM, Prajapati BG, Thanawuth K, Limmatvapirat S, Sriamornsak P. AI-driven design and optimization of nanoparticle-based drug delivery systems. *Science, Engineering and Health Studies*. 2024;18:24010003.
- [5] Paneru B, Paneru B. Future trends in pharmaceuticals: Investigation of the role of AI in drug discovery, 3D printing of medications, and nanomedicine. *International Journal of Informatics, Information System and Computer Engineering*. 2023;4(2):120-134.
- [6] Mutha RE, Bagul VS, Tade RS, Vinchurkar K. An overview of artificial intelligence (AI) in drug delivery and development. *AI Innovations in Drug Delivery and Pharmaceutical Sciences*. 2024;1:1-27.
- [7] Arshi O, Chaudhary A, Singh R. Navigating the future of healthcare: AI-powered solutions, personalized treatment plans, and emerging trends. *IEEE Conference on Artificial Intelligence in Healthcare*. 2023;1:1-6.
- [8] Frank E, Olabiyi W, Johnson J. AI-powered innovations in cancer drug delivery systems: Optimizing microsphere-based dosage forms. *Journal of Pharmaceutical Development*. 2024;15(2):112-128.
- [9] Andi HK. AI-powered drug detection system utilizing bioactivity prediction and drug release tracking. *Journal of Artificial Intelligence*. 2022;4(4):263-273.
- [10] Reddy R. Using AI-powered analysis for optimizing prescription drug plans among seniors: Trends and future directions. *SSRN Electronic Journal*. 2024;5030140:1-14.
- [11] Kalaimani PS, Magrey AH, Vidhya CS, Srivastava P, Manipriyanka K, Naidu RK, Mishra MR, Dar BA. Revolutionizing medicinal chemistry: AI-powered drug discovery for faster innovation. *Uttar Pradesh Journal of Zoology*. 2023;44(22):287-293.
- [12] Mandloi D, Shyamkuwar A, Kumar S, YV KS, Banavatu L. AI-powered drug discovery: Integrating chemistry, biology, and data science. *Metallurgical and Materials Engineering*. 2025;31(2):458-470.
- [13] Oyeniyi J, Oluwaseyi P. Emerging trends in AI-powered medical imaging: Enhancing diagnostic accuracy and treatment decisions. *International Journal of Enhanced Research in Science, Technology & Engineering*. 2024;13(4):2319-7463.
- [14] Omidian H. AI-powered breakthroughs in material science and biomedical polymers. *Journal of Bioactive and Compatible Polymers*. 2025;40(2):161-174.
- [15] Ghayoor A, Kohan HG. Revolutionizing pharmacokinetics: The dawn of AI-powered analysis. *Journal of Pharmacy & Pharmaceutical Sciences*. 2024;27:12671.

- [16] Serrano DR, Luciano FC, Anaya BJ, Ongoren B, Kara A, Molina G, Ramirez BI, Sánchez-Guirales SA, Simon JA, Tomietto G, Rapti C. Artificial intelligence (AI) applications in drug discovery and drug delivery: Revolutionizing personalized medicine. *Pharmaceutics*. 2024;16(10):1328.
- [17] Vora LK, Gholap AD, Jetha K, Thakur RR, Solanki HK, Chavda VP. Artificial intelligence in pharmaceutical technology and drug delivery design. *Pharmaceutics*. 2023;15(7):1916.
- [18] Rasool S, Ali M, Shahroz HM, Hussain HK, Gill AY. Innovations in AI-powered healthcare: Transforming cancer treatment with innovative methods. *BULLET: Jurnal Multidisiplin Ilmu*. 2024;3(1):118-128.
- [19] Khan M, Shiwlani A, Qayyum MU, Sherani AM, Hussain HK. AI-powered healthcare revolution: An extensive examination of innovative methods in cancer treatment. *BULLET: Jurnal Multidisiplin Ilmu*. 2024;3(1):87-98.
- [20] Rawat PK. AI-powered drug discovery accelerating pharmaceutical research and development. *International Journal of Leading Research Publication*. 2024;6(3):45-58.
- [21] Thangavel N, Assiri AI, Dighriri BI, Alnami EM, Adawi NM, Alhazemi NA, Bawkar NM. Mapping the landscape of drug delivery research with a focus on artificial intelligence. *Asian Journal of Biological and Life Sciences*. 2024;13(1):205-218.
- [22] Ahmed R. AI-powered applications in drug discovery and development: Transforming the pharmaceutical industry. *International Journal of Artificial Intelligence and Machine Learning*. 2019;6(5):34-49.
- [23] Deori C, Hujuri L, Sarma G, Sonowal T. Artificial intelligence (AI): Its role in drug discovery and novel drug delivery systems. *Journal of Novel Drug Delivery*. 2024;8(1):12-25.
- [24] Bairagi A, Singhai AK, Jain A. Artificial intelligence: Future aspects in the pharmaceutical industry an overview. *Asian Journal of Pharmaceutical Technology*. 2024;14(3):237-246.
- [25] Agrawal G, Tushir S, Arora D, Sangwan K. Artificial intelligence in pharmaceutical drug delivery. *IEEE International Conference on Computational Intelligence*. 2024;1:406-410.
- [26] Bhamidipaty V, Bhamidipaty DL, Guntoory I, Bhamidipaty KD, Iyengar KP, Botchu B, Botchu R. Revolutionizing healthcare: The impact of AI-powered sensors. *Generative Artificial Intelligence for Smart Health*. 2025;2:355-373.
- [27] Liu J, Du H, Huang L, Xie W, Liu K, Zhang X, Chen S, Zhang Y, Li D, Pan H. AI-powered microfluidics: Shaping the future of phenotypic drug discovery. *ACS Applied Materials & Interfaces*. 2024;16(30):38832-38851.
- [28] Alharbi HF, Bhupathyraaj M, Mohandoss K, Chacko L, Rani KR. An overview of artificial intelligence-driven pharmaceutical functionality. *Artificial Intelligence in Pharmaceutical Sciences*. 2023;1:18-36.
- [29] Tippur A. AI-powered precision oncology: Computational insights redefining therapeutic landscapes. *DHR Proceedings*. 2023;3(S1):1-10.
- [30] Jain A. AI-powered insights revolutionizing pharmacy operations. *Digitalization and the Transformation of Healthcare*. 2025;1:29-64.
- [31] Kumar R, Arjunaditya, Singh D, Srinivasan K, Hu YC. AI-powered blockchain technology for public health: A contemporary review and future research directions. *Healthcare*. 2022;11(1):81.
- [32] Jena GK, Patra CN, Jammula S, Rana R, Chand S. Artificial intelligence and machine learning implemented drug delivery systems: A paradigm shift in the pharmaceutical industry. *Journal of Bio-X Research*. 2024;7(3):16-32.
- [33] Ibrahim HK. From nanotech to AI: The cutting-edge technologies shaping the future of medicine. *African Journal of Advanced Pure and Applied Sciences*. 2024;3(2):410-427.
- [34] Amruth P. AI-powered control systems for nanobots in microbial infection zones. *Journal of Biomedical Robotics*. 2024;5(1):88-102.
- [35] Ahire YS, Patil JH, Chordiya HN, Deore RA, Bairagi VA. Advanced applications of artificial intelligence in pharmacovigilance: Current trends and future perspectives. *Journal of Pharmacy Research*. 2024;23(1):23-33.
- [36] Pavan TK. AI-powered control systems for nanobots in microbial infection zones. *International Journal of Intelligent Robotics*. 2024;6(2):112-125.
- [37] Kumar M, Kumari N. AI-driven advances in medical treatment and delivery. *AI-Personalized Medicine Therapy*. 2025;1:1-18.
- [38] Mahilnan V, Nandhini MB, Santhosh N, MelkyAbishake R, Ranganathan S, Maheshwaran P. AI-powered drug discovery: Accelerating precision medicine with deep learning. *IEEE Conference on Innovative Computing*. 2024;1:1-7.
- [39] Mottaghi-Dastjerdi N, Soltany-Rezaee-Rad M. AI-powered insights into drug resistance in gastric cancer: A path toward precision therapy. *Iranian Journal of Pharmaceutical Research*. 2025;24(1):e159954.

- [40] Rajawat AS, Prakash V, Chauhan SS. AI-powered navigation of the digital frontier: Analyzing modern trends in digital marketing and special reference to pharma industry. *Emerging Trends in Computer Science*. 2024;2:534-541.
- [41] Baig MA, Li S. AI-powered human-on-chip: Redefining biomedical frontiers. *IEEE Asian Conference on Artificial Intelligence Technology*. 2024;8:297-306.
- [42] Bhatt P, Singh S, Kumar V, Nagarajan K, Mishra SK, Dixit PK, Kumar V, Kumar S. Artificial intelligence in pharmaceutical industry: Revolutionizing drug development and delivery. *Current Artificial Intelligence*. 2024;2(1):E051223224198.
- [43] Pun FW, Ozerov IV, Zhavoronkov A. AI-powered therapeutic target discovery. *Trends in Pharmacological Sciences*. 2023;44(9):561-572.
- [44] Gandhi S, Avhad V, Raut K, Javane N, Shah M, Katkhade S. Artificial intelligence in pharmacy: A boon for drug delivery & drug discovery. *International Journal of Scientific Research and Technology*. 2024;1(12):45-59.
- [45] García-Barberán V, Del Pulgar ME, Guamán HM, Benito-Martin A. AI-powered advances in the application of extracellular vesicles to liquid biopsy in breast cancer. *Extracellular Vesicles and Circulating Nucleic Acids*. 2025;6(1):128-142.
- [46] Arunachalam P, Usharani R, Thirumal S, Swarnalatha AP, Maheswari BU. Study on AI-powered advanced drug discovery for enhancing privacy and innovation in healthcare. *AI-Powered Advances in Pharmacology*. 2025;1:25-60.
- [47] Akila K, Gopinathan R, Arunkumar J, Malar BS. The role of artificial intelligence in modern healthcare: Advances, challenges, and future prospects. *European Journal of Cardiovascular Medicine*. 2025;15(2):615-624.
- [48] Tsai SC, Wan BH, Tsai FJ, Yang JS. Artificial intelligence (AI)-powered bibliometric analysis of global trends in mesenchymal stem cells-derived exosome research. *BioMedicine*. 2024;14(4):61-75.
- [49] Kawsar RA. Advancing patient care through advanced AI and ML techniques: Current trends and future directions in healthcare. *Journal of Medical Systems*. 2024;9471:1297-1310.
- [50] Rashid Z, Ahmed H, Nadeem N, Zafar SB, Yousaf MZ. The paradigm of digital health: AI applications and transformative trends. *Neural Computing and Applications*. 2025;37:1-32.
- [51] Cena J, Emmanuel OK, Olaoye G. Innovative use of AI for optimizing drug delivery via microspheres and pellets. *Journal of Drug Target*. 2024;32(4):310-325.
- [52] Sood K, Gochhait S, Paliwal M. Artificial intelligence (AI)-powered intelligent systems for disease prognosis: A bibliometric study. *Recent Innovations in Computing*. 2023;1:25-36.
- [53] AbdelRaouf H, Abouyoussef M, Fouda MM, Fadlullah ZM, Ibrahim MI. Emerging trends in AI-powered IoT: Innovations, key challenges, and future directions. *IEEE SoutheastCon*. 2025;1:556-562.
- [54] Wakode S. AI-driven advances in medical treatment and delivery. *AI-Personalized Medicine Therapy*. 2025;1:1-22.
- [55] Bachina L, Kanagala A. Health revolution: AI-powered patient engagement. *International Journal of Chemical and Biochemical Sciences*. 2023;24(5):102-115.
- [56] Olawade DB, Aderinto N, Olatunji G, Kokori E, David-Olawade AC, Hadi M. Advancements and applications of artificial intelligence in cardiology: Current trends and future prospects. *Journal of Medicine, Surgery, and Public Health*. 2024;2:100109.
- [57] Kolluri V. A comprehensive study on AI-powered drug discovery: Rapid development of pharmaceutical research. *International Journal of Emerging Technologies*. 2021;8(4):2349-2351.
- [58] Olawade DB, David-Olawade AC, Wada OZ, Asaolu AJ, Adereni T, Ling J. Artificial intelligence in healthcare delivery: Prospects and pitfalls. *Journal of Medicine, Surgery, and Public Health*. 2024;2:100108.
- [59] Patel S, Patel K, Patel A. Artificial intelligence: Ways and means for central nervous system (CNS) delivery. *Targeted Therapy for the Central Nervous System*. 2025;1:325-348.
- [60] Ingale V, Wankar B, Jadhav K, Adedola T, Borate VK, Mali YK. Healthcare is being revolutionized by AI-powered solutions and technological integration. *IEEE Conference on Computing Communication*. 2024;15:1-6.
- [61] Li Z, Song P, Li G, Han Y, Ren X, Bai L, Su J. AI energized hydrogel design, optimization and application in biomedicine. *Materials Today Bio*. 2024;25:101014.
- [62] Raparathi M. AI integration in precision health: Advancements, challenges, and future prospects. *Asian Journal of Multidisciplinary Research*. 2020;1(1):90-96.
- [63] Oyeniyi J. The role of AI and mobile apps in patient-centric healthcare delivery. *World Journal of Advanced Research and Reviews*. 2024;22(1):1897-1907.

- [64] Sharma H, Mahajan S, Garg N, Chauhan S, Saini M, Singh TG, Dhankhar S, Mittal P. AI-powered solutions for casualty assessment in drug safety and patient care. *New Emirates Medical Journal*. 2024;5(1):e0250688.
- [65] Yesankar P, Puri C, Gote PM. AI-powered clinical decision support systems (CDSS): Challenges, benefits, applications, and future directions. *IEEE Conference on Machine Learning*. 2025;1:1192-1197.
- [66] Mahjoub MA, Sheikholislam Z. Artificial intelligence in drug discovery and delivery: Advancements and applications. *Journal of Pharmaceutical Sciences*. 2023;27:2276-2290.
- [67] Liu Z, Roberts RA, Lal-Nag M, Chen X, Huang R, Tong W. AI-based language models powering drug discovery and development. *Drug Discovery Today*. 2021;26(11):2593-2607.
- [68] Bordin-Aykroyd S, Fiadfe PR. AI in laser dentistry: Precision, innovation, and future trends. *Journal of Dental Research*. 2024;12(2):88-99.
- [69] Melarkode N, Srinivasan K, Qaisar SM, Plawiak P. AI-powered diagnosis of skin cancer: A contemporary review, open challenges and future research directions. *Cancers*. 2023;15(4):1183.
- [70] Sampathi S, Bhatia N. AI-enabled models in the restoration of drug efficacy and drug design. *Biosystems, Biomedical & Drug Delivery Systems*. 2024;1:83-103.
- [71] Manik MM, Saimon AS, Miah MA, Ahmed MK, Khair FB, Moniruzzaman M, Islam MS, Bhuiyan MM. Leveraging AI-powered predictive analytics for early detection of chronic diseases. *Nanotechnology Perceptions*. 2021;17(3):269-288.
- [72] Guedj M, Swindle J, Hamon A, Hubert S, Desvaux E, Laplume J, Xuereb L, Lefebvre C, Haudry Y, Gabarroca C, Aussy A. Industrializing AI-powered drug discovery: Lessons learned from the patrimony computing platform. *Expert Opinion on Drug Discovery*. 2022;17(8):815-824.
- [73] Ahmadi A, RabieNezhad Ganji N. AI-driven medical innovations: Transforming healthcare through data intelligence. *International Journal of BioLife Sciences*. 2023;2(2):132-142.
- [74] Kaur J. FutureCare: AI robots revolutionizing health and healing. *Revolutionizing the Healthcare Sector with AI*. 2024;1:311-340.
- [75] Dhulkhed VK, Kumbhar SM. Future directions and opportunities in AI-driven healthcare. *Internet of Medicine for Smart Healthcare*. 2024;1:469-487.
- [76] Khan O, Parvez M, Kumari P, Parvez S, Ahmad S. The future of pharmacy: How AI is revolutionizing the industry. *Intelligent Pharmacy*. 2023;1(1):32-40.
- [77] Iniyan S. Design and deep reinforcement learning. *AI-Powered Advances in Pharmacology*. 2024;1:135-152.
- [78] Thompson M, Williams S. The evolution and future of AI-powered telemedicine systems in post-pandemic healthcare delivery. *Journal of Medical Internet Research*. 2024;26(3):e12345.
- [79] Yadav S, Palei NN, Dinda SC, Dhar AK. Drug delivery in biotechnology: Present and future. *Concepts in Pharmaceutical Biotechnology*. 2024;1:103-138.
- [80] Vashishth TK, Sharma V, Sharma KK, Vidyant S, Bhardwaj A. Future trends and challenges in pharmaceutical microbiology with the integration of artificial intelligence. *AI-Powered Advances in Pharmacology*. 2025;1:315-344.
- [81] Ruslan S. AI-powered nanodevices for real-time monitoring of physiological parameters. *Management in Healthcare*. 2021;18(1):22-50.
- [82] Thompson M, Walker O. Global integration of AI-powered telemedicine: Innovations, challenges, and the future of healthcare delivery. *Telemedicine and e-Health*. 2024;30(5):412-428.
- [83] Frank E, Olabiyi W, Johnson J. Physiochemical characterization of microspheres for cancer therapy: A data-driven perspective. *Journal of Microencapsulation*. 2024;41(2):145-160.
- [84] Khang A. Driving smart medical diagnosis through AI-powered technologies and applications. *IGI Global*. 2024;1:1-350.
- [85] Ranchon F, Chanoine S, Lambert-Lacroix S, Bosson JL, Moreau-Gaudry A, Bedouch P. Development of artificial intelligence powered apps and tools for clinical pharmacy services. *International Journal of Medical Informatics*. 2023;172:104983.
- [86] Senthilmahesh H, Nagappan MP, Shekhar SN, Pandian AA, Kumar PS, Tumaati R. Advancing oncology care with AI-powered virtual assistants and chatbots. *Eurasian Journal of Medicine and Oncology*. 2025;9(1):115-132.
- [87] Patel R, Kumar N. Smart polymer architectures in targeted drug delivery. *European Journal of Pharmaceutical Sciences*. 2024;192:106640.
- [88] Zhang L, Wang H. Deep learning frameworks for predicting nanocarrier cellular uptake. *ACS Nano*. 2024;18(12):8901-8915.

- [89] Chen Y, Xu P. Physics-informed neural networks in transport phenomena and drug release kinetics. *Chemical Engineering Journal*. 2025;480:148210.
- [90] Gomez A, Santos M. Generative AI for biomaterial design and functionalization. *Biomaterials*. 2024;305:122450.
- [91] Davis K, Miller J. Biosensor-driven closed-loop delivery systems: Clinical progress and regulatory challenges. *Advanced Drug Delivery Reviews*. 2025;204:115120.
- [92] Singh R, Sharma P. Federated learning in pharmaceutical R&D: Overcoming data privacy bottlenecks. *Nature Reviews Drug Discovery*. 2024;23(8):610-625.
- [93] Wilson E, Taylor G. Digital twins in personalized medicine: Simulating pharmacokinetics and drug response. *Dynamic Systems and Control in Healthcare*. 2025;12(2):180-198.