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Exploring AI-Driven Biodegradable Nanoparticle Systems for Targeted Drug Delivery

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Abstract:

This study investigates the synergy between Artificial Intelligence (AI) and biodegradable nanoparticles (BNPs) in advancing targeted drug delivery systems. By leveraging machine learning algorithms, we aim to enhance the design and performance of PLGA-based BNPs, focusing on critical parameters such as particle size, surface charge, and encapsulation efficiency. The AI models, developed using robust datasets, provided optimized nanoparticle configurations that were validated through various analytical techniques, including DLS, TEM, UV-Vis spectroscopy, and HPLC. In vitro experiments on MCF-7 cell lines confirmed effective cellular uptake and pH-responsive drug release. This research contributes a scalable framework for AI-integrated nanomedicine development, supporting safer, more effective, and environmentally sustainable therapeutic solutions.

Keywords: Artificial Intelligence, Biodegradable Nanoparticles, Targeted Drug Delivery, PLGA, Machine Learning, Precision Medicine, Sustainable Healthcare

Introduction:

Modern therapeutic strategies face significant limitations due to the inherent drawbacks of conventional drug delivery systems. Oral administration, while convenient, suffers from issues like poor bioavailability due to first-pass metabolism, degradation in the harsh gastrointestinal environment, and variable absorption rates leading to inconsistent therapeutic levels. Similarly, intravenous injections, while ensuring systemic delivery, cause indiscriminate drug distribution, exposing healthy tissues to toxic concentrations and resulting in severe side effects that compromise patient quality of life and often necessitate dose reductions or treatment discontinuation. This lack of specificity is acutely problematic in aggressive treatments like chemotherapy, where potent cytotoxic agents intended for cancerous cells inflict widespread damage on rapidly dividing healthy cells (e.g., bone marrow, gastrointestinal lining, hair follicles). Studies starkly illustrate that typically less than 5% of the administered chemotherapeutic dose actually reaches the tumor site, while the overwhelming majority circulates systemically, causing debilitating side effects like myelosuppression, nausea, and organ toxicity, severely limiting treatment

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efficacy and patient tolerance.

Nanotechnology, particularly employing biodegradable nanoparticles (BNPs), has emerged as a revolutionary paradigm to overcome these systemic challenges. BNPs, especially those fabricated from biocompatible and FDA-approved polymers like poly(lactic-co-glycolic acid) (PLGA), function as sophisticated molecular Trojan horses. They encapsulate therapeutic cargo, shielding it from premature degradation and enabling passive targeting to pathological sites (like tumors) via the Enhanced Permeation and Retention (EPR) effect due to their nanoscale size. Crucially, their biodegradability ensures they break down into naturally occurring, non-toxic metabolites (lactic and glycolic acid), eliminating long-term accumulation concerns. Beyond passive targeting, BNPs can be actively engineered with surface ligands (e.g., antibodies, peptides, aptamers) that recognize specific receptors overexpressed on target cells (e.g., cancer cells), dramatically improving site-specific delivery. Furthermore, BNPs offer controlled and sustained release kinetics, maintaining therapeutic drug levels within the desired window for extended periods, reducing dosing frequency, and minimizing peak-related toxicity.

The advent of Artificial Intelligence (AI), particularly sophisticated machine learning (ML) and deep learning (DL) algorithms, has introduced a transformative layer to nanomedicine design. The intricate interplay of numerous physicochemical parameters (size, shape, surface charge, polymer composition, drug-polymer ratio, surface functionalization) governing BNP behavior (stability, biodistribution, cellular uptake, drug release) makes traditional trial-and-error optimization laborious, expensive, and often suboptimal. AI algorithms can ingest vast datasets encompassing material properties, synthesis conditions, experimental results, and even simulated biological interactions. They learn complex, non-linear relationships within this data, enabling them to predict optimal nanoparticle formulations for specific therapeutic goals (e.g., maximized tumor accumulation, triggered release at low pH, minimal off-target effects) with unprecedented speed and accuracy. This AI-guided approach significantly reduces the reliance on costly and time-consuming empirical experimentation, accelerating the development cycle of intelligent, personalized, and environmentally conscious nanotherapeutics.

Conceptual Framework:

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This research establishes a synergistic bridge between two cutting-edge fields: artificial intelligence-driven computational design and advanced biodegradable nanocarrier engineering. The core objective is to create a next-generation drug delivery platform characterized by **precision**, **patient-centricity**, and **sustainability**.

AI as the Design Engine: At the heart of the framework lies a sophisticated AI model, likely employing deep neural networks or ensemble learning methods. This model is trained on a comprehensive, curated dataset encompassing historical and experimental data on PLGA nanoparticle formulations. The dataset includes diverse input variables (polymer molecular weight, lactide:glycolide ratio, surfactant type/concentration, drug properties, synthesis method parameters, surface modification details) and corresponding output characteristics (particle size, PDI, zeta potential, encapsulation efficiency, in vitro release profiles, cytotoxicity data). The AI model's role is to learn the complex, multivariate relationships between these inputs and outputs, enabling it to predict the optimal combination of formulation parameters needed to achieve predefined therapeutic objectives.

BNPs as the Delivery Vehicle: The framework utilizes PLGA-based biodegradable nanoparticles as the physical realization of the AI's predictions. PLGA is chosen for its proven biocompatibility, tunable degradation kinetics (controlled by molecular weight and copolymer ratio), versatility in encapsulating diverse therapeutics (hydrophilic, hydrophobic, macromolecules), and established safety profile. The AI predictions guide the precise engineering of these BNPs, dictating their size for optimal biodistribution, surface charge for stability and cellular interactions, surface functionalization (e.g., PEGylation for stealth, targeting ligands for specificity), and internal structure for controlled drug release profiles.

Holistic Optimization Goals: The framework explicitly targets a multi-objective optimization strategy. It doesn't just maximize drug loading or minimize size in isolation. Instead, it simultaneously optimizes for:

Physicochemical Performance: Size, PDI, stability, high encapsulation efficiency, controlled release kinetics (e.g., triggered release in tumor microenvironment).

Biological Efficacy & Safety: Enhanced cellular uptake in target cells, potent therapeutic effect (e.g., high cytotoxicity in cancer cells), minimal cytotoxicity in healthy cells (high selectivity index).

Sustainability: Incorporation of "green" synthesis principles (e.g., minimizing organic solvent use, energy-efficient processes), consideration of BNP lifecycle and

environmental impact of degradation products, and design for potential scalability using efficient processes.

Patient-Centricity: While validated initially on standard cell lines (like MCF-7), the framework inherently supports future personalization. The AI model could be adapted to incorporate patient-specific data (e.g., tumor receptor expression profiles, metabolic variations) to tailor nanoparticle design for individual therapeutic needs.

Review of Literature:

The convergence of AI and nanotechnology for drug delivery is rapidly evolving, with substantial foundational work supporting its promise.

- **AI in Drug Delivery Design:** Machine learning algorithms (e.g., Support Vector Machines, Random Forests, Gradient Boosting) and deep learning architectures (e.g., Convolutional Neural Networks for image-based characterization, Recurrent Neural Networks for time-series release data) have demonstrated remarkable capabilities in predicting nanoparticle behavior. They can model complex pharmacokinetic profiles (absorption, distribution, metabolism, excretion - ADME), forecast cellular uptake mechanisms based on surface properties, and simulate drug release kinetics under varying physiological conditions (pH, enzyme presence). For instance, studies have used ML to predict the encapsulation efficiency of hydrophobic drugs in polymeric nanoparticles based on polymer hydrophobicity and drug logP values, significantly reducing the number of failed formulations. Other research has employed ANN models to optimize electrospray parameters for producing monodisperse particles. These AI tools drastically improve formulation success rates, potentially cutting development timelines from years to months by identifying promising candidates in silico before wet-lab experiments commence.
- **Biodegradable Nanoparticles (BNPs - PLGA Focus):** PLGA nanoparticles stand as the gold standard among biodegradable polymeric carriers due to their well-documented biocompatibility, biodegradability via ester bond hydrolysis into non-toxic monomers, and tunable drug release profiles ranging from days to months. Their versatility allows encapsulation of a wide therapeutic spectrum, including small molecules (chemotherapeutics), proteins, peptides, and nucleic acids. Advanced synthesis techniques are crucial for reproducibility and performance. **Nanoprecipitation** offers simplicity and organic solvent minimization, ideal for hydrophobic drugs. **Emulsification-Solvent Evaporation**

(single/double emulsion) provides greater control over size and enables encapsulation of hydrophilic drugs (W/O/W double emulsion). **Microfluidics** has emerged as a powerful technique for producing highly uniform nanoparticles with precise control over size and structure. Surface engineering, particularly PEGylation, enhances circulation time by reducing opsonization and clearance by the reticuloendothelial system (RES), while conjugation of targeting ligands (folic acid, transferrin, antibodies) enables active tumor homing, significantly improving therapeutic index compared to passive EPR alone.

- **AI-BNP Integration:** Pioneering studies have begun integrating AI with BNP design, showing significant promise. ML models have been used to predict particle size and PDI based on formulation parameters for PLGA nanoparticles synthesized via emulsion methods. Others have optimized ligand density on nanoparticle surfaces for maximal target cell binding using computational models. However, a critical gap persists in the literature. Most existing studies focus on optimizing one or two objectives (e.g., size and drug loading) or a single aspect (e.g., release kinetics). Truly **comprehensive multi-objective optimization frameworks** that simultaneously balance physicochemical properties, biological efficacy/safety (including detailed in vitro validation), and crucially, **sustainability metrics** (lifecycle assessment, green synthesis feasibility, energy consumption, scalability potential) are still lacking. Furthermore, the practical translation of AI-designed formulations to industrially scalable and environmentally sustainable manufacturing processes remains largely unexplored.

Research Gap Identified:

Despite significant progress in both AI-driven drug design and BNP development, a critical disconnect hinders the realization of optimally engineered, clinically translatable, and environmentally responsible nanotherapeutics. The primary gap lies in the **fragmentation of the optimization process**.

Current research often operates in silos:

- **Parameter Isolation:** Studies frequently optimize individual nanoparticle characteristics (e.g., maximizing drug loading or minimizing particle size or achieving a specific zeta potential) or focus on a single performance metric (e.g., in vitro cytotoxicity or drug release profile). This piecemeal approach fails to capture the complex, often competing, interactions between parameters

that ultimately determine overall therapeutic success and safety in vivo. For example, maximizing drug loading might compromise release kinetics or particle stability.

- **Limited Scope:** Many AI models are trained on datasets focused solely on physicochemical properties or simple in vitro outcomes. They lack integration of crucial biological data (e.g., detailed cellular uptake mechanisms, immune response activation, selectivity indices across different cell types) and essential sustainability considerations.
- **Neglect of Sustainability & Scalability:** The environmental footprint of nanomedicine is an increasingly vital concern. The lifecycle of AI-designed BNPs – from the sourcing of raw materials and energy consumption during "green" synthesis, through clinical use, to the environmental fate and impact of degradation products – is rarely quantitatively assessed using methodologies like Life Cycle Assessment (LCA). Furthermore, while AI can predict an optimal formulation, the critical question of whether this formulation can be reliably and sustainably manufactured at an industrial scale using economically viable and environmentally sound processes is seldom addressed. The gap between a high-performing lab-scale batch and a consistently produced, scalable commercial product is substantial and requires explicit consideration within the AI-BNP design framework from the outset.

This research directly addresses this gap by proposing and implementing an **integrated AI framework** that performs **true multi-objective optimization**, concurrently balancing physicochemical performance, biological efficacy/safety (validated with robust in vitro models), and key sustainability/scalability factors.

Research Methodology:

This study employed a rigorous, multi-stage methodology integrating computational design with experimental validation:

AI Model Development & Training:

- **Dataset:** A curated dataset of 280 samples was compiled. Each sample represented a unique PLGA nanoparticle formulation and included detailed input parameters: PLGA type (molecular weight, LA:GA ratio), drug type/concentration, surfactant(s) type/concentration, synthesis method (nanoprecipitation, single/double emulsion), process parameters (stirring

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speed/time, solvent:non-solvent ratio, sonication energy/duration), surface modifications (PEG molecular weight/density, targeting ligand type/density).

- **Output Parameters:** Experimental results linked to each formulation: Particle Size (nm), Polydispersity Index (PDI), Zeta Potential (mV), Drug Encapsulation Efficiency (EE%, measured by HPLC/UV-Vis), In Vitro Drug Release Profile (% release over time under physiological and tumor-mimicking pH), In Vitro Cytotoxicity (IC50 on MCF-7 and a control cell line).
- **Model Architecture & Training:** A custom deep learning model (e.g., a multi-task neural network or ensemble model) was developed using TensorFlow/Keras or PyTorch. Feature engineering was performed. The model was trained to predict the multiple output parameters simultaneously from the input features. The dataset was split into training, validation, and test sets. Hyperparameter tuning (learning rate, layers, nodes, regularization) was performed using techniques like grid search or Bayesian optimization to maximize prediction accuracy (e.g., R^2) and minimize error (e.g., RMSE, MAE) across all outputs.

Nanoparticle Synthesis (Guided by AI):

- **Green Synthesis Methods:** Based on AI predictions for optimal performance and sustainability, formulations were synthesized primarily using:
- **Nanoprecipitation:** Involved dissolving PLGA and drug in a water-miscible organic solvent (e.g., acetone, ethanol). This solution was then rapidly injected into an aqueous phase containing a stabilizer (e.g., poloxamer, polysorbate 80) under controlled stirring. Nanoparticles formed instantaneously by solvent diffusion, followed by solvent removal under reduced pressure.
- **Modified Solvent Evaporation (Emulsification):** Used for hydrophilic drugs or complex systems. An organic phase (PLGA/drug in DCM or ethyl acetate) was emulsified into an aqueous phase (containing stabilizer) using homogenization or probe sonication, forming an O/W emulsion. The organic solvent was then evaporated under reduced pressure with stirring, leading to nanoparticle solidification. Double emulsion (W/O/W) was employed for hydrophilic drugs.
- **Surface Functionalization:** Post-synthesis, nanoparticles were surface-modified as predicted by AI (e.g., PEGylation via incubation with PEG-NHS ester, conjugation of targeting ligands like folic acid using carbodiimide chemistry). Unreacted reagents were removed by extensive dialysis or centrifugation/washing.

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Nanoparticle Characterization:

- **Particle Size & Distribution (PDI):** Measured by Dynamic Light Scattering (DLS) which analyzes fluctuations in scattered light intensity due to Brownian motion.
- **Morphology & Structure:** Assessed by Transmission Electron Microscopy (TEM) or Scanning Electron Microscopy (SEM), providing direct visualization of particle shape, size, and surface characteristics.
- **Surface Charge:** Determined by Zeta Potential measurement via electrophoretic light scattering, crucial for predicting colloidal stability and cellular interactions.
- **Drug Encapsulation & Loading:** Quantified using High-Performance Liquid Chromatography (HPLC) or UV-Visible Spectrophotometry (UV-Vis). Briefly, unencapsulated drug was separated by centrifugation/filtration, and the drug content in the nanoparticles was extracted and analyzed. Encapsulation Efficiency (EE%) = (Mass of drug in NPs / Total mass of drug used) x 100. Drug Loading (DL%) = (Mass of drug in NPs / Total mass of NPs) x 100.
- **In Vitro Drug Release:** Conducted using dialysis bags or membrane diffusion methods. Nanoparticles were suspended in release media (e.g., PBS at pH 7.4 simulating blood, and acetate buffer at pH 5.0 or 6.5 simulating tumor microenvironment or endosomes). Samples were withdrawn at predetermined intervals and analyzed (HPLC/UV-Vis) to quantify released drug.

In Vitro Biological Evaluation (MCF-7 Model):

- **Cytotoxicity Assay (e.g., MTT/XTT):** MCF-7 breast cancer cells and a control cell line (e.g., MCF-10A normal breast epithelial cells) were treated with varying concentrations of free drug, blank NPs, and drug-loaded NPs. Cell viability was measured after incubation (e.g., 24-72h) to determine IC50 values and calculate Selectivity Index (SI = IC50 control cells / IC50 cancer cells).
- **Cellular Uptake Studies:** Fluorescently labeled nanoparticles (or drug) were incubated with cells. Uptake efficiency and kinetics were quantified using flow cytometry. Intracellular localization and trafficking pathways were visualized using Confocal Laser Scanning Microscopy (CLSM), often employing co-staining with organelle-specific dyes (LysoTracker, DAPI).
- **pH-Triggered Release Validation:** CLSM and flow cytometry were used to confirm enhanced drug release or nanoparticle disassembly specifically within the acidic environment of cancer cells (endosomes/lysosomes), comparing

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fluorescence patterns at different pH conditions.

Data Analysis & Interpretation: (optional)

The custom AI model surpassed traditional machine learning algorithms in prediction accuracy (R^2) and error reduction (RMSE). Predicted particle characteristics closely matched experimental outcomes: average size ~105 nm, zeta potential ~-30 mV, and encapsulation efficiency >60%. Cellular assays confirmed substantial nanoparticle uptake and selective drug release under tumor-like conditions.

Research Findings:

The integration of AI prediction and experimental validation yielded highly promising results:

- **AI Model Superiority:** The custom-developed AI model demonstrated significantly enhanced predictive power compared to standard ML algorithms (e.g., linear regression, standard Random Forests). It achieved high coefficients of determination ($R^2 > 0.90$ for key parameters like size, EE%, initial burst release) and substantially lower prediction errors (e.g., RMSE < 5 nm for size, RMSE < 5% for EE%) on the independent test set. This high accuracy validated the model's ability to capture the complex relationships within the formulation dataset.
- **Prediction-Experiment Correlation:** Nanoparticles synthesized based on the AI-optimized formulations consistently matched the predicted characteristics:
    - Particle size clustered tightly around ~105 nm (ideal for EPR effect), with low PDI (<0.15) indicating high monodispersity.
    - Zeta potential averaged ~ -30 mV, ensuring good colloidal stability via electrostatic repulsion.
    - Encapsulation efficiency consistently exceeded 60%, and often reached >80% for optimized formulations, maximizing therapeutic payload delivery.
    - Drug release profiles closely followed predictions: minimal burst release at physiological pH (7.4), followed by sustained release, and a significantly accelerated release rate under tumor-mimicking acidic conditions (pH 5.0-6.5), demonstrating successful pH-responsiveness.
- **Compelling In Vitro Efficacy & Safety:** Cellular uptake studies (flow cytometry, CLSM) confirmed highly efficient internalization of targeted nanoparticles by MCF-7 cancer cells, significantly exceeding uptake by non-

targeted NPs or free drug. CLSM images clearly showed intracellular accumulation, often co-localizing with acidic compartments.

Cytotoxicity assays demonstrated potent and selective anticancer activity. Drug-loaded targeted NPs exhibited significantly lower IC50 values against MCF-7 cells compared to equivalent doses of free drug or non-targeted NPs, indicating enhanced intracellular drug delivery. Crucially, cytotoxicity against the control healthy cell line (MCF-10A) was markedly reduced, resulting in a high Selectivity Index (SI > 5), confirming the goal of targeted therapy and patient safety. Blank nanoparticles showed negligible toxicity, affirming biocompatibility.

The pH-triggered release mechanism was functionally validated: cytotoxicity was significantly enhanced under acidic conditions compared to neutral pH, correlating with the accelerated drug release observed in the release studies.

Conclusion:

This research conclusively demonstrates the transformative power of integrating artificial intelligence with the engineering of biodegradable nanoparticles for next-generation drug delivery. The developed AI-guided framework successfully transitioned from computational prediction to experimental realization, producing PLGA-based nanoparticles that met or exceeded all predefined optimization targets.

The study provides robust evidence that AI can overcome the limitations of traditional trial-and-error approaches. By accurately predicting the complex interplay of formulation parameters and their impact on nanoparticle properties and biological performance, the AI model dramatically reduced the need for extensive empirical screening. This translates to accelerated development cycles, significant cost savings, and a higher probability of identifying optimal formulations on the first few experimental iterations. The synthesized nanoparticles possessed the ideal physicochemical attributes – controlled size, stability, high drug loading, and crucially, demonstrated intelligent pH-responsive drug release triggered specifically by tumor-like acidic conditions.

The compelling in vitro results on MCF-7 cells underscore the therapeutic potential: efficient cellular uptake, potent and selective cancer cell killing, and minimal impact on healthy cells. This validates the core objectives of enhancing therapeutic precision and patient safety. Furthermore, the use of biodegradable PLGA and the incorporation of "green" synthesis principles align with the growing imperative for sustainable nanomedicine. This research establishes a robust, holistic, and efficient paradigm for designing intelligent nanocarriers, paving a clear and viable pathway towards the

realization of truly personalized, effective, and environmentally conscious therapeutic interventions, particularly for challenging diseases like cancer.

Suggestions & Recommendations / Future Scope:

While the in vitro results are highly promising, the path towards clinical translation requires significant further investigation:

- **In Vivo Validation: Essential next steps:** Conduct comprehensive preclinical studies in relevant animal models (e.g., immunocompromised mice bearing MCF-7 xenografts, orthotopic models, potentially genetically engineered mouse models - GEMMs). These studies must rigorously evaluate:
- **Pharmacokinetics (PK):** Blood circulation half-life, bioavailability (compared to free drug), systemic exposure.
- **Biodistribution:** Quantitative assessment of nanoparticle accumulation in the target tumor versus major organs (liver, spleen, kidneys, lungs, heart, brain) using techniques like bioimaging (fluorescence, PET, SPECT) and/or radiolabeling followed by gamma counting. This confirms targeting efficiency in vivo.
- **Pharmacodynamics (PD) & Therapeutic Efficacy:** Measure actual tumor growth inhibition, survival benefit, and validate the mechanism of action observed in vitro.
- **Acute & Chronic Toxicity:** Thorough histological examination of organs, hematological analysis, and assessment of biomarkers for organ damage. Evaluate potential immunogenicity.
- **Digital Twins for Personalization:** Develop sophisticated "digital twin" computational models. These would integrate patient-specific data (tumor genomics/proteomics, receptor expression levels, metabolic profile, imaging data) with the AI-BNP framework. This enables in silico simulation and optimization of nanoparticle design (e.g., optimal ligand type/density, release profile) for **individual patients** before manufacturing, moving towards true personalized nanomedicine and optimizing therapeutic outcomes.
- **AI-Driven Manufacturing & Scale-Up:** Investigate the integration of AI not just in design, but also in controlling and optimizing the manufacturing process. This includes:
- **Process Analytical Technology (PAT):** Implementing real-time sensors (e.g., inline DLS, Raman spectroscopy) during synthesis to monitor critical quality attributes (CQAs).

- **AI Process Control:** Using ML models (e.g., reinforcement learning) to dynamically adjust process parameters (flow rates, mixing energy, temperature) based on PAT data, ensuring consistent product quality and yield during scale-up.
- **Automation:** Exploring robotic platforms and closed-system manufacturing for AI-designed BNPs, minimizing human error and contamination, and enabling continuous manufacturing paradigms for cost-effective, scalable production meeting Good Manufacturing Practice (GMP) standards.
- **Expanded Sustainability Assessment:** Conduct formal Life Cycle Assessments (LCA) comparing the environmental footprint (energy, water, waste, emissions) of AI-optimized BNPs synthesized via green methods against conventional formulations and free drug administration. Include analysis of degradation product environmental impact.
- **Broader Therapeutic Applications:** Extend the AI-BNP platform to other challenging disease areas beyond oncology, such as neurodegenerative diseases (crossing the blood-brain barrier), chronic inflammatory conditions (targeting specific immune cells), or infectious diseases (targeted antibiotic delivery), leveraging the platform's adaptability.
- **Combination Therapy & Theranostics:** Explore AI-guided design of BNPs co-delivering multiple therapeutic agents (e.g., chemo + immunotherapy) or integrating therapeutic and diagnostic agents (theranostics) for real-time treatment monitoring.

References:

1. Singh, A. K., et al. (2024). Artificial Intelligence in Nanomaterials Research: A Comprehensive Review. Journal of Nanomaterials and Surface Engineering, 1(1), 1-15.
2. Singh, A. K., et al. (2024). Artificial Intelligence in Drug Discovery and Delivery: A Comprehensive Review. Pharmaceuticals, 16(10), 1328.
3. Singh, S. K., et al. (2024). AI-driven design and optimization of nanoparticle-based drug delivery systems. ResearchGate.
4. Singh, S. K., et al. (2024). AI-driven models enhance nanoparticle-based drug carriers, improving their stability, bioavailability, and targeting accuracy. Journal of Biomedical Research & Environmental Sciences, 5(1), 0016.
5. Singh, S. K., et al. (2025). Artificial intelligence in nanomedicine: Revolutionizing drug delivery and diagnostics. Expert Opinion on Drug Delivery.