AI Powered Target Cancer Drug Delivery System

Khushi Sharma, Rohit Jain, Annu Rajput,

Department of pharmacy,

Ch. Sughar Singh Pharmacy College, Jaswant Nagar, India.

Abstract: Biochemical guidelines, AI, and targeted medications are critical to contemporary oncology. To avoid cell-death marker overlaps, autophagy monitoring requires targeting many genes and verifying different assays. Standard chemotherapies for gastric cancer shorten overall survival to 8–11 months as compared to colorectal treatments. Conversely, natural beta-glucans are potent immunomodulators that significantly improve survival in melanoma (HR 0.65) and lung cancer (HR 0.72) when paired with PD-1 inhibitors. Concurrently, deep learning optimizes photodynamic therapy, achieving 90–95% accuracy in adaptive dosage tumor diagnosis. Strict laboratory standards, state-of-the-art biotherapeutics, and AI algorithmic precision are all at the forefront of tailored cancer treatment.

Keywords: precision oncology, autophagy, gastric cancer, photodynamic therapy, artificial intelligence, and beta-glucans**.**

1.INTRODUCTION

The process of transporting and releasing a pharmaceutical ingredient at the proper location within the body to have the intended therapeutic effect is known as drug delivery. A drug's pharmacological activity, absorption, distribution, metabolism, excretion, and capacity to reach the target tissue all affect how effective it is. When a medication is administered conventionally, the active pharmaceutical ingredient is often distributed throughout the body rather than just at the site of sickness. This non-specific distribution may enhance side effects and decrease treatment efficacy.

As a result, tailored drug delivery systems (TDDS) have become a crucial tactic for enhancing treatment results. Increasing medication concentration at the intended biological location while reducing exposure to healthy tissues is the goal of targeted delivery. Passive processes, active ligand-mediated mechanisms, or stimuli-responsive strategies can all be used to accomplish targeting. For this reason, research on nanoparticles, liposomes, polymeric micelles, dendrimers, lipid nanoparticles, and other nanocarriers is growing.

Drug bioavailability, targeting, dose-response properties, and therapeutic effectiveness can all be enhanced by nanomedicines; yet, their development is complicated because to the interplay between several formulation and biological factors. Conventional formulation development frequently relies on optimization and repetitive testing. This kind of trial-and-error can be costly and time-consuming.

An alternate data-driven strategy is provided by artificial intelligence. AI is described by the U.S. Food and Drug Administration (FDA) as machine-based systems that may make suggestions, forecasts, or judgments based on predetermined goals. One of the main AI techniques employed in the pharmaceutical industry is machine learning. The FDA has seen an increase in the use of AI components in the manufacturing, post-marketing, clinical, and nonclinical phases of the drug product life cycle.

Therefore, the rational design of delivery systems can be made easier by integrating AI with targeted medicine delivery. Computational models can anticipate promising combinations of medication, carrier, excipient, targeted ligand, and process parameters without the need to test a large number of formulations empirically. AI-guided formulation creation may enhance the prediction and optimization of crucial quality parameters such particle size, drug encapsulation, drug loading, and drug release, according to recent research.

2. The idea of targeted medication delivery

A pharmaceutical strategy known as "targeted drug delivery" involves delivering a medication specifically to the intended place of action. An organ, tissue, sick cell, receptor, or intracellular space could be the target.

Targeted delivery's main goal is to accomplish:

- ✓ Drug concentration at the target location has increased.
- ✓ Decreased drug levels in healthy tissues
- ✓ Enhanced efficacy of treatment
- ✓ Decreased toxicity in the body
- ✓ Sustained or regulated medication release
- ✓ Increased adherence to treatment

Passive and active targeting are two general categories of targeted delivery.

2.1 Non-Active Targeting

The natural distribution and physiological traits of a carrier determine passive targeting. Changes in vascular permeability, blood flow, and tissue architecture may lead nanoparticles to collect preferentially in some sick tissues.

A number of physicochemical and biological factors affect how effective passive targeting is. AI can help analyze these data and forecast how various nanoparticle compositions will likely be distributed.

2.2 Intentional Targeting

By adding molecules that can identify particular receptors or biomarkers to a drug carrier, active targeting is accomplished. Targeting molecule examples include:

1. Antimicrobials
2. Sequences
3. Aptamers, Folate, and Carbs
4. Ligands unique to a receptor

AI may be useful for optimizing carrier properties, predicting ligand-receptor interactions, and locating appropriate target receptors.

3. Artificial Intelligence's Function in Medication Administration

The development of medicine delivery can use artificial intelligence at several phases. Large datasets from biological research, imaging, molecular databases, pharmaceutical tests, and clinical studies can all be processed by it.

The following is an illustration of a streamlined AI-assisted medicine distribution workflow:

Data gathering → Data processing → AI model creation → Forecasting → Optimization of formulations → Validation thru experiments → Final delivery system.

AI models may use data such as:

- ✓ Properties of drugs' physiochemistry
- ✓ Features of lipids and polymers
- ✓ Composition of formulations
- ✓ Particle dimensions
- ✓ Surface electricity
- ✓ Encapsulation effectiveness
- ✓ Capacity to load drugs
- ✓ Drug-release information
- ✓ Stability information
- ✓ Pharmacokinetic specifications
- ✓ Expression of the receptor
- ✓ Properties of tissues

The model gains knowledge of the connections between input variables and intended results. Following validation, it can be applied to forecast how new formulations will behave
The multifaceted nature of drug delivery systems makes this strategy very helpful. A little modification to one formulation variable might have a simultaneous impact on multiple other qualities.

4. Key AI Technologies for Targeted Drug Delivery

4.1 Intelligent Learning

In pharmaceutical research, machine learning (ML) is one of the most significant AI technologies. In order to forecast future data, machine learning algorithms utilize patterns they discover in preexisting datasets.

Typical ML techniques consist of:

- ✓ Regression that is linear
- ✓ A woodland at random
- ✓ Tree of decisions
- ✓ Vector machine support

Bayesian modeling, gradient boosting, and k-nearest neighbor
For instance, previously created nanoparticle formulations with data on medication concentration, polymer concentration, surfactant concentration, and preparation conditions can be used to train an ML model. For a fresh formulation, the trained model can then forecast encapsulation efficiency or particle size.
Applications of machine learning (ML) in various nanoparticulate systems and in the prediction of crucial quality features such as particle size, surface characteristics, encapsulation efficiency, drug loading, drug release, and stability have been documented in recent reviews.

4.2 Neural Network Artificial Systems

Computational models called artificial neural networks (ANNs) draw inspiration from biological neural networks. They typically have three layers: input, concealed, and output.
ANNs are especially helpful in nonlinear relationship analysis. Several formulation factors may interact nonlinearly in medication distribution. As a result, features including particle size, drug release, encapsulation efficiency, and stability can be predicted using ANNs.

4.3 In-depth Education

A specific area of machine learning built on multilayer neural networks is called deep learning. Large and complicated datasets benefit greatly from it.

Potential uses for targeted medication administration consist of:

- ✓ Image-based study of cells
- ✓ Analysis of nanoparticles
- ✓ Molecular property forecasting
- ✓ Predicting drug-target interactions
- ✓ Forecasting biodistribution
- ✓ Evaluation of biological reactions

Additionally, deep learning has the ability to analyze medical images and possibly detect disease-related traits that can direct the choice of targeted delivery methods.

4.4 Natural Language Interpretation

Computers can analyze human language thanks to natural language processing, or NLP. Large volumes of data are produced by pharmaceutical research and are stored in databases, scientific articles, patents, and clinical reports.

Researchers can benefit from NLP in:

- ✓ Looking up scientific literature
- ✓ Information extraction from formulations
- ✓ Determining drug-target associations
- ✓ Evaluating patents
- ✓ Arranging scientific information
- ✓ Structure of scientific knowledge
- ✓ Creating datasets that are structured

This can assist researchers find previously reported correlations between medications, carriers, and targeted techniques and shorten the time needed for literature analysis.

4.5 Bayesian Adjustment

Formulation development is frequently an optimization problem with multiple variables. In order to determine the next experimental condition that is likely to yield valuable information, Bayesian optimization makes use of prior experimental outcomes.
For instance, Bayesian optimization can offer viable formulation conditions if a researcher wishes to improve encapsulation efficiency while preserving a particular particle size and controlled release profile.
This could lessen the quantity of experimental batches needed to develop a formulation**.**

4.6 Artificial Intelligence and Inverse Design

Conventional pharmaceutical formulation typically takes a proactive approach:

- ✓ Performance → Properties → Formulation

This process may be reversed by AI:

- ✓ Ideal characteristics → Anticipated composition

Researchers might, for instance, designate a desirable drug-loading capacity, release profile, and particle size. Then, an AI model can recommend a formulation composition that might accomplish those qualities.
Predictive or inverse formulation design, as opposed to trial-and-error development, is thot to be a significant future path for AI-assisted medicine delivery.

5. AI in Targeted Drug Delivery using Nanoparticles

One of the most researched delivery systems for tailored medication is nanoparticles. Drug loading, release, biodistribution, and cellular uptake can all be controlled by altering their characteristics.

Important systems based on nanoparticles consist of:

- ✓ Polymer-based particles
- ✓ The liposomes
- ✓ Lipid-based particles
- ✓ Lipid solid nanoparticles
- ✓ Carriers of nanostructured lipids
- ✓ Microscopic polymers
- ✓ Hybrid nanoparticles, dendrimers, nano emulsions, and nanocrystals

These systems' production circumstances and composition can be optimized with the use of AI. ML applications across various nanoparticulate delivery systems were compiled in a recent review that was published in Acta Pharmaceutica Sinica B. The review emphasized ML's capacity to predict significant quality aspects.

5.1 Particle Size Prediction

Biodistribution, cellular uptake, stability, and drug-release behavior can all be impacted by particle size. AI models can forecast particle size prior to experimental preparation by analyzing formulation and process variables.
This can make it easier for researchers to find appropriate formulation conditions**.**

5.2 Encapsulation Efficiency Prediction

The percentage of medication that is successfully integrated into a delivery vehicle is known as encapsulation efficiency.
Drug characteristics, carrier makeup, preparation technique, and processing conditions all have an impact. AI is able to estimate the anticipated encapsulation efficiency and identify correlations between these factors.

5.3 Drug Release Prediction

Particle size, polymer degradation, drug solubility, carrier composition, and environmental factors all affect drug release.
AI is able to forecast release profiles by analyzing these variables. This could aid in the creation of controlled-release and sustained-release systems.

5.4 Stability Forecast

For drug delivery to be successful, both chemical and physical stability are crucial. AI may be able to determine connections between formulation composition and stability results and assist in the selection of more stable formulations.

6. Using AI to Optimize Ligands and Select Targets

Finding the right biological target is necessary for effective active targeting. The target should ideally be reachable by the delivery system and adequately expressed at the illness site.
AI can find possible targets by analyzing biological and molecular databases. Additionally, drug-target and ligand-receptor interactions can be predicted with the use of machine learning.
For instance, a delivery system intended for cancer treatment might employ a ligand against a receptor that is highly expressed on particular tumor cells. Using the biological data that is now available, AI may assist in comparing potential receptors and ligands.
Optimizing ligand density on the surfaces of nanoparticles may also be aided by AI. Targeting, stability, or cellular interactions may be adversely affected by an excessive or insufficient ligand density. In order to determine an appropriate range prior to experimental testing, computational optimization may be helpful.

7. Personalized Drug Delivery Using AI

The goal of personalized medicine is to choose a course of treatment based on each patient's unique traits. Genetics, metabolism, disease stage, receptor expression, and pharmacokinetic behavior can all vary greatly among patients.

AI is capable of combining various patient-related datasets, such as:

- ✓ Genome-related data
- ✓ Clinical facts
- ✓ Pharmacokinetic data with imaging data
- ✓ Symptoms of the disease
- ✓ Expressed biomarkers
- ✓ This makes it possible to develop more customized drug-delivery plans.

An AI-supported system might help choose a carrier with a ligand targeted at a particular receptor, for instance, if that receptor is highly expressed in a patient's tumor.
The combination of AI with nanomedicine may open up possibilities for patient-specific medicinal approaches, even if such personalized targeted delivery is still a developing field.
8. Drug Delivery Applications for Cancer
Because traditional anticancer medications may harm both malignant and healthy cells, cancer is one
Anticancer medications may be better distributed and have regulated or targeted release thanks to nanocarriers.

AI can help distribute cancer medications in the following ways:

- ✓ Finding cancer-related targets
- ✓ Predicting interactions between drugs and targets
- ✓ Choosing systems for nanocarriers
- ✓ Enhancement of nanoparticle composition
- ✓ Estimation of medication release
- ✓ Estimate of biodistribution
- ✓ Imaging analysis of tumors
- ✓ Creation of Customized Treatment Approaches

Tumor traits and cellular properties that are important for targeting may be identified with the aid of AI-based image analysis. Integrating clinical and molecular data is another application of machine learning.
Nevertheless, clinical efficacy cannot be determined by computational prediction alone. Before being used to therapeutic decisions, AI-generated predictions must undergo experimental, preclinical, and clinical validation.

9. Benefits of AI-Powered Targeted Medication Administration

Compared to strictly traditional formulation development, AI offers a number of possible benefits.

9.1 A decrease in trial-and-error

Many experimental batches may be necessary for the creation of a traditional formulation. Before laboratory testing, AI can determine formulation circumstances that show promise.

9.2 Optimizing Formulations More Quickly

AI is capable of quickly analyzing various formulation combinations and forecasting their potential results.

9.3 Better Prognosis

Complex and nonlinear correlations between performance and formulation variables can be found using machine learning.

9.4 Effective Use of Information

AI can be used to systematically analyze large volumes of biological and pharmacological data.

9.5 Potential Cost Cutting

The time and resources needed for formulation development could be decreased by reducing pointless experiments.

9.6 Assistance for Customized Counseling

AI can incorporate patient-specific data and possibly facilitate customized medication distribution plans.

9.7 Better Nanocarrier Architecture

AI can assist in improving aspects like medication loading and release, surface features, and particle size.

10. Difficulties and Restrictions

Despite its potential, AI-powered tailored medicine delivery is not widely used due to a number of obstacles.

10.1 Limited High-Quality Data Availability

AI models need adequate and trustworthy datasets. Pharmaceutical datasets may be produced using various experimental techniques, be tiny, or be incomplete.

10.2 Data Uniformity

When assessing particle size, medication loading, release, or stability, different labs may employ different techniques. The trustworthiness of pooled datasets may be lowered by such variations.

10.3 Issue with Black-Box

Certain sophisticated AI models make extremely accurate predictions, but they don't explain how they were made. Pharmaceutical research may suffer from a lack of interpretability.

10.4 Biological Intricacy

Human biological systems are incredibly intricate. A model that was developed using data from laboratories might not be able to predict human behavior.

10.5 Experimental Verification

Experimental validation is required for AI predictions. It's possible that a computationally anticipated formulation won't behave the same way in a lab or clinical setting.

10.6 The ability to repeat

AI performance can change based on the model architecture, training settings, dataset, and algorithm. Thus, it is crucial to use reproducible research methods.

10.7 Regulatory Unpredictability

Regulators require proof that AI models are trustworthy for the particular applications for which they are designed. A risk-based credibility evaluation approach for AI models used to assist regulatory decisions concerning pharmaceutical or biological goods is proposed in the FDA's 2025 draft guidance.

10.8 Concerns about Privacy and Ethics

Data security and privacy must be upheld when using patient data in AI development. Ethical measures and proper governance are required.

11. Regulatory Issues

The need for suitable regulatory frameworks has arisen from the growing application of AI in pharmaceutical research.
The FDA has released guidelines and principles pertaining to appropriate AI use and has documented an increase in the use of AI components in medication development. Ten guiding principles for effective AI practice in drug development were established by the FDA and the European Medicines Agency (EMA) in January 2026. Human-centric design, risk-based methods, a clear context of usage, interdisciplinary knowledge, data governance, model development, performance evaluation, and lifecycle management are some of these.

Key regulatory factors for AI-powered targeted medication distribution could be:

- ✓ A precise description of the intended use of the AI model
- ✓ Data quality and traceability
- ✓ Validating models appropriately
- ✓ Evaluation of model functionality
- ✓ Supervision by humans
- ✓ Recording the creation of the model
- ✓ Monitoring following execution
- ✓ reproducibility of the findings

The regulatory environment is changing as AI applications spread throughout the life cycle of pharmaceutical products. The FDA now acknowledges the use of AI in nonclinical research, clinical development, manufacturing, and post-marketing operations.
Pharmaceutical scientists should therefore take regulatory regulations into account from the outset of their research when creating AI-enabled delivery systems.

12. Looking Ahead

A deeper integration of AI, nanotechnology, automation, and experimental pharmaceutics is probably in store for AI-powered tailored medicine delivery in the future.
One significant advancement is the idea of automated or "self-driving" labs. In these systems, artificial intelligence (AI) can recommend an experiment, automated lab equipment can carry it out, and the data collected can be put back into the model. The freshly created data can then be used by the model to choose the subsequent experiment.

One way to depict the procedure is as:

- ✓ AI prediction → Data creation → Automated experiment → Model updating → Better prediction

Combining machine learning with models based on mechanisms and physiology is another exciting avenue. When there aren't enough experimental datasets, these hybrid methods could enhance prediction.
Predicting the pharmacokinetics and biodistribution of nanoparticles may also be a growing use of AI. This is especially crucial because it is challenging to forecast nanoparticle distribution, aggregation, and clearance using traditional techniques.
As a result, future tailored medication delivery systems might become more individualized, adaptable, and predictive. However, multidisciplinary cooperation amongst pharmacists, pharmaceutical scientists, biologists, nanotechnologists, physicians, data scientists, and regulatory specialists will be necessary for successful translation.

13. AI's Potential Impact on Pharmaceutical Science

Instead, then taking the place of pharmaceutical experts, AI is predicted to have an impact on their roles. Formulation scientists and pharmacists will need to be aware of how AI models are created, verified, and analyzed.

Future pharmacists could have to:

- ✓ Recognize fundamental machine learning and artificial intelligence ideas.
- ✓ Assess the dataset's quality.
- ✓ Interpret predictions made by AI
- ✓ Construct experimental validation studies
- ✓ Improve drug formulations
- ✓ Examine stability and safety.
- ✓ List the limitations of the model.
- ✓ Preserve adherence to regulations

Thus, fundamental understanding of AI can become more and more important for Pharm students. Students may be better prepared for the future pharmaceutical industry by integrating data science, computational modeling, and artificial intelligence with courses like pharmaceutics, pharmacology, and pharmaceutical chemistry.

14. Final Remarks

AI-powered targeted medicine delivery is a new multidisciplinary strategy that combines biological sciences, pharmaceutical sciences, nanotechnology, and artificial intelligence. By enhancing drug exposure at the intended site while lowering exposure to healthy tissues, targeted drug delivery seeks to increase the therapeutic index of medications.

Different phases of drug delivery development can benefit from AI technologies as machine learning, artificial neural networks, deep learning, natural language processing, Bayesian optimization, and generative techniques. In addition to helping with target identification, ligand optimization, biodistribution prediction, and customized therapy, they can predict particle size, encapsulation efficiency, drug loading, drug release, and stability.
Because the effectiveness of nanoparticulate delivery systems depends on a variety of interrelated formulation and biological factors, they provide a very significant field for AI application. The use of machine learning for formulation design, optimization, and characterization of various nanoparticle-based delivery systems has garnered increasing attention, according to recent study.

AI shouldn't be seen as a replacement for experimental science, nevertheless. Restrictions pertaining to biological complexity, repeatability, interpretability, standardization, data quality, and regulatory constraints need to be addressed. Human supervision and proper experimental validation are still crucial.

All things considered, AI has the ability to change targeted medication administration from a mostly trial-and-error method to one that is more predictive and data-driven. The transfer of AI-designed delivery systems from lab research to clinical applications might be accelerated by ongoing development of high-quality datasets, explainable AI, automated experimentation, and suitable regulatory frameworks.

Allusions

Food and Drug Administration, United States. The use of artificial intelligence in drug development. The FDA...
Food and Drug Administration, United States. The fundamentals of ethical AI practice in drug development. Jan. 2026.
Food and Drug Administration, United States. A Look at Artificial Intelligence's Potential to Help with Drug and Biological Product Regulation Decision-Making. Draft Policy, January 2025.
Current uses, difficulties, and prospects for the design, development, and characterization of nanoparticulate drug delivery systems enabled by machine learning. Acta Pharmaceutica Sinica B. 16(2):665–685. 2026.