

## Chapter 11: Role of Artificial Intelligence and Machine Learning in Advancing Nanomedicine for Breast Cancer Therapy

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### Abstract

Breast cancer is still one of the most common and serious cancers that affect women globally. The standard treatments have deficiencies like non-personalization, drug resistance, and off-target toxicity. Therefore the Nanotechnology-based treatments hold a promising alternative. These technologies provide increased bioavailability, diminished systemic toxicity and drug targeting. But due to the complexity in the biology of tumors and patient heterogeneity, there is a requirement of adaptive and smart solutions. Artificial intelligence (AI) and machine learning (ML) with nanotechnology has emerged as a game-changer in the treatments of the breast cancer. This chapter explores the potential of AI and ML in nanotechnology-based approaches in advancing Nanomedicine for breast cancer therapy. This advancement improves the treatment of breast cancer and increases the survival rate. It includes deep learning, and predictive modeling strategies which are helpful in drug release kinetics, nanoparticle design, and personal treatment planning. The focus is on real-time monitoring of therapeutic responses, biomarker discovery, and AI-based diagnostic systems. Although multiple advantages, there are some challenges such as data insufficiency, model interpretability, ethical issues, and nanotoxicity which are also discussed in this chapter. Real-world applications and case studies are also discussed to depict the industrial application of the technology. The convergence can potentially radically change breast cancer treatments using the artificial intelligence technologies to implement personalized and optimized treatment.

**Keywords:** *Artificial Intelligence, Breast Cancer, Machine Learning, Nanomedicine, Nanotechnology, Therapy*

## 1. Introduction

The breast cancer is the most common cancer detected in women worldwide based on the research conducted by Sung *et al.*, 2021. Despite the major developments, the traditional therapies like chemotherapy, radiation, and surgery have drawbacks which include systemic toxicity, lack of target specificity, and the emergence of multidrug resistance as observed by Wang *et al.*, 2016 in his research work. Nanotechnology can overcome these drawbacks with improved treatment and rapid recovery using engineered nanoparticles based on the research by Bobo *et al.*, 2016.

Artificial intelligence (AI) and machine learning (ML) have the enhanced capabilities of drug development. They provide personalized treatment planning, and diagnostics. These technologies analyze high-dimensional biomedical data to make predictions as per the research by Esteva *et al.*, 2019. The research by You *et al.*, 2022 states that AI and ML are helpful in optimizing nanoparticle design, forecast drug release profiles, and customize therapeutic regimens. AI and ML in convergence with nanotechnology brought a paradigm shift in the treatment of breast cancer. They have the potential for achieving personalized and highly targeted treatments.

This chapter aims to explore the technological developments, clinical applications, and future research directions in the treatment of the breast cancer.

## 2. Fundamentals of Nanotechnology in Breast Cancer

Nanotechnology enhances the efficacy and specificity of drug delivery and reduces systemic toxicity. As per the research by Peer *et al.*, 2007, the nanocarriers overcome the limitations such as non-specific biodistribution, rapid drug elimination, and drug resistance, thus facilitating targeted delivery of chemotherapeutic agents to the tumor tissue.

### 2.1 Nanocarriers and Nanoformulations

Nanocarriers are basically specific designed materials that are typically 1 to 100 nanometers in diameter. The nanocarriers are helpful in the treatment of the breast cancer by releasing the therapeutic drug in a regulated way. The most commonly utilized ones are liposomes, dendrimers, polymeric nanoparticles, and inorganic nanoparticles as per the research by Shi *et al.*, 2017.

These nanostructures can be ligand or antibody functionalized for the purpose of increasing their selective internalization by cancer cells according to the work of Wilhelm *et al.*, 2016.

## **2.2 Passive vs. Active Targeting in Tumor Microenvironment**

There are two main methods used in nanomedicine such as passive and active targeting, where passive targeting utilizes the enhanced permeability and retention (EPR) effect, which happens when tumors have leaky vasculature that allows nanoparticles to accumulate preferentially (Maeda *et al.*, 2000) and active targeting, involves surface modifications of nanoparticles with targeting moieties such as folic acid, HER2 antibodies, or peptides that bind to specific receptors over expressed in breast cancer cells (Danhier *et al.*, 2010).

## **2.3 Types of Nanoparticles Used in Breast Cancer Therapy**

Numerous nanoparticles have been explored for breast cancer therapy. Liposomes like Doxil® (pegylated liposomal doxorubicin) are FDA-approved and have demonstrated reduced cardiotoxicity compared to free doxorubicin (Barenholz, 2012). Polymeric nanoparticles release polymers like Chitosan and PLGA (poly (lactic-co-glycolic acid)), are biodegradable in nature. According to Jain *et al.*, 2012, metal-based nanoparticles particularly gold nanoparticles are being researched for their potential uses in photothermal therapy and diagnostics because of their optical characteristics and simplicity of functionalization.

## **2.4 Benefits of Nanotechnology-Based Approaches**

Nanotechnology has a number of benefits over conventional chemotherapy, such as increased drug solubility, defense against enzymatic breakdown, extended half-life, and fewer adverse effects. Torchilin, 2014 states that the nanoparticles are versatile enough to enable imaging in response to internal or external stimuli such as temperature, pH, and magnetic fields.

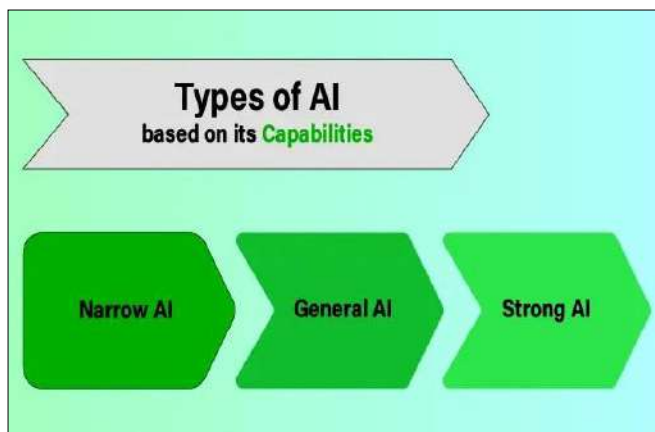
These features result in better treatment of breast cancer, especially triple-negative breast cancer (TNBC) as per the research by Rosenblum *et al.*, 2018.

## **3. Artificial Intelligence and Machine Learning: Concepts and Relevance**

Artificial intelligence (AI) and machine learning (ML) support the breast cancer treatment by providing strong tools. These tools are helpful for processing large datasets, creating predictive models, and analytical decision-making. According to the research by Jiang *et al.*, 2017, AI and ML are improving diagnosis, optimizing nanoparticle design, customizing treatments, and enhancing clinical outcomes in nano-based breast cancer therapeutics.

### **3.1 Introduction to Artificial Intelligence**

The artificial intelligence (AI) consists of systems which have the ability to learn, reason, and solve problems. The objective of AI is to develop machines that can perform functions similar to human beings. Perception, analysis, and language understanding are some such tasks (Russell & Norvig, 2020). There are three broad types of AI which are, Narrow AI, General AI, and Strong AI. Fig. 11.1 shows how AI is categorized.



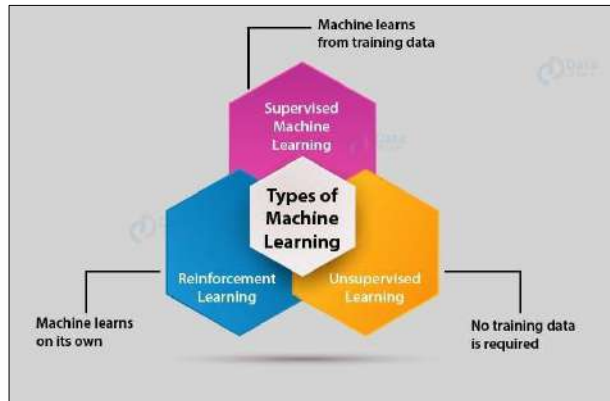
**Fig.11.1** AI Categorization

- Narrow AI: Made to carry out particular tasks, like mammography image recognition.
- General AI refers to hypothetical systems that are capable of carrying out any intellectual task that a human is capable of.
- Strong AI vs. Weak AI: Strong AI refers to machines with conscious intelligence (still theoretical), while Weak AI focuses on task-specific problem-solving using algorithms.

In healthcare, AI enables predictive analytics, diagnostic support, treatment personalization, and real-time monitoring, particularly beneficial when managing complex diseases like breast cancer.

### 3.2 Introduction to Machine Learning (ML)

A branch of artificial intelligence called machine learning aims to create systems that can learn from data and enhance performance without the need for explicit programming (Jordan & Mitchell, 2015). In order to generate predictions or judgments, machine learning algorithms look for patterns in datasets. According to LeCun, Bengio, and Hinton (2015), machine learning algorithms can be divided into three categories: supervised learning (such as regression and classification), unsupervised learning (such as clustering), and reinforcement learning. Fig. 11.2 shows the different forms of machine learning.



**Fig. 11.2** Forms of Machine Learning

Different forms of machine learning are explained below:

**a. Supervised Learning**

- Requires labeled datasets.
- Algorithms learn from input-output pairs to predict outcomes (e.g., classifying tumors as benign or malignant).
- Support Vector Machines (SVM), Random Forest, Decision Trees, Neural Networks, and Logistic Regression are examples of common algorithms.
- Typically applied for drug response prediction and tumor classification (Kourou *et al.*, 2015).

**b. Unsupervised Learning**

- Applies unlabeled data to reveal patterns or underlying structure (e.g., cluster patients by genomic profiles).
- Typical algorithms include Principal Component Analysis (PCA), Hierarchical Clustering, and K-means.
- Facilitates the stratification of patient populations or the discovery of new cancer subtypes.

**c. Reinforcement Learning**

- Agents pick up knowledge through interacting with their surroundings and getting feedback in the form of rewards or penalties.

- Adaptive therapy design and optimization are increasingly using reinforcement learning, due to its more recent use in medical applications (Yu *et al.*, 2021).
- Useful in optimizing treatment plans or drug release profiles in smart nanocarriers.

### 3.3 Deep Learning in Biomedical Imaging and Drug Discovery

A sophisticated machine learning method referred to as "deep learning" utilizes multi-layered artificial neural networks. Deep learning has surpassed image recognition, natural language processing, and genomics according to the work of LeCun, Bengio, and Hinton (2015). Deep learning, particularly convolutional neural networks (CNNs), have revolutionized medical image result in high-precision tumor detection from mammograms and histopathological images, according to Esteva *et al.*, 2019. And according to another study, drug discovery, molecular simulation, and nanoparticle design optimization use generative adversarial networks (GANs) and recurrent neural networks (RNNs) (Zhavoronkov *et al.*, 2019).

### 3.4 AI and ML Tools and Platforms in Healthcare

Several open-source software such as TensorFlow, PyTorch, Scikit-learn, and Google AutoML make it easy to use AI and ML in the healthcare sector. The research by (Topol, 2019) illustrates that these software are helpful in clinical research; image analysis, risk prediction and biomarker identification. In nanomedicine, ML is used for modeling nanoparticle-biological interactions, cytotoxicity prediction, and high-throughput screening of potential formulations. It has been found that artificial intelligence (AI) and machine learning (ML) have their potential in clinical medicine and biomedical research by providing tools useful in cognitive processing and data-based decision-making.

To understand the potential, applications and limitations, it is very important to know the fundamental concepts of artificial intelligence (AI) and machine learning (ML) in the context of nanotechnology-based breast cancer treatments.

The combination of nanotechnology with AI and ML has provided a basis for precision oncology via the establishment of targeted therapies enabling real-time, patient-specific decision-making.

### 3.5 Key Concepts of AI and ML for Nanomedicine Applications

- **Feature Engineering:** Choosing and shaping data features (e.g., nanoparticle size, zeta potential) that influence model accuracy.

- **Model Training and Validation:** The data is divided into training and test sets to estimate the model’s generalizability.
- **Underfitting and Overfitting:** Underfitting is a common condition where a model is under specified and overfitting is a condition where a model is learning the noise and not the pattern.
- **Explainable AI (XAI):** Makes AI decisions interpretable and transparent to clinicians, increasing trust and adoption in clinical settings.
- **Transfer Learning:** Reuses pre-trained models on new but related tasks, which are valuable in nanomedicine, where labeled data may be scarce.

Table 11.1 shows the key AI and ML concepts for Nanomedicine.

**Table 11.1** AI and ML Concepts for Nanomedicine

Concept	Description	Relevance to Nanomedicine
Feature Engineering	Selecting and converting pertinent data features (such as surface chemistry, zeta potential, and nanoparticle size)	Enhances model performance by identifying which nanomaterial properties most influence drug delivery and therapeutic outcomes
Model Training and Validation	Splitting data into training and testing sets to develop and evaluate the model’s performance	Ensures the AI/ML models generalize well to unseen clinical and experimental nanomedicine data
Underfitting/ Overfitting	Underfitting: Model too simple to capture patterns; Overfitting: Model captures noise	Critical to avoid misleading predictions in nanotherapeutic design and efficacy analysis
Explainable AI (XAI)	Techniques to make AI models' decisions understandable to human users	Helps clinicians interpret why specific nanoparticle formulations are recommended, fostering trust in AI-generated insights
Transfer Learning	Applying insights from one model or task to a related but distinct task with sparse data	Useful in nanomedicine where annotated datasets are limited, allowing reuse of models trained on similar biomedical data

### **3.6 Importance of AI and ML in Nanotechnology-Based Breast Cancer Therapy**

- **Prediction of Nanoparticle Behavior:** ML algorithms can predict how nanoparticles will act around cancer cells.
- **Optimization of Drug Formulations:** AI can rapidly identify the most effective nanoparticle compositions.
- **Integration with Omics Data:** AI enables the synthesis of data from genomics, proteomics, and metabolomics for holistic cancer profiling.
- **Adaptive Therapy:** ML enables real-time adjustments in treatment based on patient response.

## **4. AI and ML in Breast Cancer Diagnosis and Prognosis**

Diagnosis and prognosis of breast cancer are heavily dependent on proper histopathological interpretation, molecular markers, and medical imaging. Traditional methods of diagnosis are low in sensitivity for early detection, time-consuming to interpret, and inter-observer variable. AI and ML have been revolutionizers in overcoming all these drawbacks by giving accurate and automatic decision-making (Dheeba *et al.*, 2014).

### **4.1 Deep Learning Based Image Diagnosis**

Deep learning algorithms particularly convolutional neural networks (CNNs) are of immense utility in mammogram, ultrasound, and magnetic resonance imaging (MRI) diagnosis of early breast cancer (Kooi *et al.*, 2017). Artificial intelligence-based computer-aided detection (CAD) systems have been found to have superior screening results than an expert radiologist (Rodriguez-Ruiz *et al.*, 2019).

### **4.2 Predictive Modeling of Tumor Growth and Metastasis**

ML algorithms are utilized in predictive modeling of tumor growth and metastasis. ML models predict the behavior of tumor and its recurrence risk. These models work on patients data to predict the risk of tumor recurrence (Cruz & Wishart, 2006). By this predictive analysis, personalized treatment and the identification of high-risk cases can be enhanced.

### **4.3 Biomarker Discovery and Genomic Data Analysis**

Machine learning (ML) approaches are very helpful in biomarker discovery and genomic data analysis. ML techniques such as random forests, support vector machines (SVMs), and deep autoencoders are being employed for this purpose as per the research by Wang



*et al.*, 2018. AI in integration with omics data improves the detection of cancer types and develops nanotherapies.

#### **4.4 Early Detection Using AI-Enhanced Screening Techniques**

AI-enhanced screening techniques improve early detection rates and reduce false positives; thus enhance outcomes. AI-powered algorithms trained on large datasets detect cancer in digital mammograms, thermograms, and liquid biopsies with high precision (Yala *et al.*, 2019). Also the integration of AI into wearable biosensors results in constant observation of high-risk populations.

### **5. AI and ML in Nano-Based Drug Design and Delivery**

AI and ML techniques are very helpful in nanotechnology-based drug design and delivery. These techniques optimize drug delivery systems based on nanotechnology for breast cancer. The integration of machine learning (ML) and artificial intelligence (AI) is transforming this field. According to the research by Chen *et al.*, 2021, these technologies result in design optimization, quick screening, and predictive modeling; thus speeds up the development process.

#### **5.1 AI-Guided Design of Nanocarriers**

AI and ML techniques are employed in the design of nanocarriers. They help design by analyzing experimental data and simulating physicochemical interactions. The machine learning algorithms are helpful in predicting the nanoparticle properties; reducing cytotoxicity, and increasing cellular uptake (Tiwari *et al.*, 2022). Also the support vector machines (SVMs) are helpful in the creation of nanoparticle protein corona, which has a major impact on immunological response and biodistribution.

#### **5.2 ML Models for Drug Loading and Release Kinetics**

One of the greatest challenges that Nanomedicine faces is controlled and regulated drug release at the tumor site. Machine learning models have addressed this issue. Such models are utilized in predicting drug-nanoparticle binding affinity, encapsulation efficiency, and release under physiological conditions. Deep learning models in particular recurrent neural networks (RNNs) are used to simulate temporal release profiles as well as to design optimized surface modifications or polymer formulations (Patra *et al.*, 2018).

#### **5.3 Dosage Optimization and Toxicity Minimization**

Artificial intelligence-based optimization models are being employed to balance therapeutic effectiveness with safety. Bayesian techniques and genetic algorithms are being used to maximize nanoparticle dosage and minimize toxicity (Tambe *et al.*, 2020).

AI models trained on preclinical data or patient-derived xenografts provide personalized dose recommendations.

#### **5.4 Real-Time Monitoring of Therapeutic Response**

The therapeutic response in real-time can be tracked with the help of smart nanocarriers. Machine learning techniques provide their support in modifying the treatment in real-time. These trained models analyze the patient data to provide the results. The research by Singh *et al.* (2020) says that AI-based nanorobots can modulate the release of drugs on the basis of tumor microenvironmental cues. The integration of AI and ML is beneficial in enhancing the outcome of treatment and safety of the patient.

The fusion of AI, ML and nanomedicine has brought a revolution in patient-specific drug delivery platforms for the treatment of breast cancer.

### **6. AI/ML in Personalized Nanomedicine for Breast Cancer**

AI and ML integration gives more personalized Nanomedicine for breast cancer. The focus is to individualize treatment plans in terms of patient's specific traits. For example, the research by Mirnezami *et al.*, 2012 states that the fusion of AI/ML techniques with nanomedicine is transforming the treatment of breast cancer by making highly individualized treatment plans. AI models trained with large imaging, genomic and clinical data sets are useful in the design, selection, and deployment of nanoformulations tailored to the unique tumor features of an individual patient.

#### **6.1 Patient Stratification and Risk Assessment**

Individualized treatment is initiated through patient subgroups and their personalized molecular profiles. Machine learning methods such as k-means clustering and hierarchical clustering classify patients from transcriptomic and proteomic information (Shah *et al.*, 2021). These patient subgroups are indeed personalized breast cancer subtypes like HER2-positive, triple-negative, or luminal A/B. These subtypes differ in terms of their predictability, management, and aptness for nanotherapy.

#### **6.2 AI-Powered Decision Support Systems for Treatment Planning**

AI-powered clinical decision support systems (CDSS) assist oncologists in the application of nanoformulation-based therapies based on patient-specific parameters (comorbidities, tumor load, and gene expression profiles). The systems predict the likely efficacy and toxicity of treatment regimens and thus reduce the risk of overtreatment or under treatment (Topol, 2019).

#### **6.3 Integration of Omics Data for Personalized Nanotherapy**

Personalized nanotherapy is obtained by the huge amount of “omics” data (genomics, transcriptomics, proteomics, and metabolomics). Omics data is served as a rich source for personalizing nanomedicine. ML models help to identify novel therapeutic targets and biomarkers. Deep learning models such as autoencoders and graph neural networks help to extract pertinent patterns from intricate biological networks; devising patient-specific drug delivery frameworks using nanoparticles (Zhang *et al.*, 2020).

#### **6.4 Feedback Loops for Adaptive Treatment Strategies**

AI/ML technologies in combination with nanomedicine are very beneficial to modify the breast cancer treatment in real-time. Smart nanocarriers equipped with sensors are able to track biological feedback indicators, tumor response, and medication release. As per the research by Abdullah *et al.* (2021), the AI models are used to adjust dosing schedules, drug combinations, or nanoparticle composition based on the patient data. These closed-loop adaptive systems prove as a key development in the treatment of breast cancer.

### **7. Nanotechnology-Based Approaches for Breast Cancer Treatment**

Because nanotechnology offers extremely accurate, regulated, and customized drug delivery systems, it has become a ground-breaking platform in the treatment of cancer. Nanotechnology makes it possible to create nanoparticles that can selectively target tumor cells, reduce off-target toxicity, and react to the tumor microenvironment in breast cancer treatments. Combining these methods with AI and ML can optimize them for better therapeutic results.

#### **7.1 Overview of Nanotechnology-Based Oncology**

Materials and devices with dimensions in the nanometer range (1-100 nm) are engineered and used in nanotechnology. Because of their small size and high surface area-to-volume ratio, nanoparticles can be functionalized for targeted therapy, accumulate in tumor tissues through the enhanced permeability and retention (EPR) effect, and cross biological barriers (Patra *et al.*, 2018).

#### **7.2 Types of Nanocarriers Used in Breast Cancer Therapy**

Types of nanocarriers used in breast cancer therapy include liposomes, polymeric nanoparticles, metallic nanoparticles, dendrimers and carbon-based nanomaterials. Table 2 shows different types of nanocarriers with their applications in breast cancer therapy.

**Table 11.2** Nanocarriers Used in Breast Cancer Therapy

Nanocarrier Type	Description	Example	Applications in Breast Cancer	Reference
Liposomes	Lipid bilayer vesicles capable of encapsulating both hydrophilic and hydrophobic drugs	Doxil® (liposomal doxorubicin)	Used for targeted chemotherapy and reduced toxicity	Barenholz, 2012
Polymeric Nanoparticles	Biocompatible and biodegradable particles (e.g., PLGA) that can respond to pH, temperature, or enzymatic changes in tumors	PLGA nanoparticles	Controlled release, site-specific delivery, stimuli-responsive therapy	Tambe <i>et al.</i> , 2020
Metallic Nanoparticles	Gold, silver, and iron oxide nanoparticles act as drug carriers and imaging agents	Gold nanoparticles	Photothermal therapy, imaging, and combination therapy	Khatoon <i>et al.</i> , 2021
Dendrimers	Highly branched, treelike nanostructures with large surface area for drug attachment	PAMAM dendrimers	High drug loading, multivalent targeting, gene/drug delivery	Kesharwani <i>et al.</i> , 2014
Carbon-Based Nanomaterials	Carbon nanotubes and graphene derivatives with unique mechanical/electrical properties	Carbon nanotubes, graphene oxide	Drug delivery, photothermal therapy, multifunctional platforms	Chung <i>et al.</i> , 2013

### 7.3 Functionalization for Targeted Therapy

Different methods are being employed to surface-modify the nanoparticles. These are as illustrate below:

- Monoclonal antibodies (e.g., anti-HER2) are being used to target overexpressed receptors in breast cancer.
- Peptides or aptamers for ligand-receptor-mediated delivery.
- Polyethylene glycol (PEG) for stealth properties to evade immune clearance.

Targeted delivery helps in reducing systemic toxicity, enhancing accumulation in tumor tissue by sparing healthy cells and thus improving therapeutic efficacy (Patra *et al.*, 2018).

## 7.4 Stimuli-Responsive Nanocarriers

The intelligent systems release medications due to certain internal stimuli (such as an acidic pH, enzymes, or redox potential) or external triggers (such as light, heat, or a magnetic field). AI-powered algorithms are used to optimize these release mechanisms to enhance the accuracy (Wang *et al.*, 2022).

## 7.5 Theranostic Nanoparticles

Theranostic nanoparticles are helpful in real-time imaging, drug delivery monitoring, and treatment efficacy assessment by combining therapeutic and diagnostic properties. For example iron oxide nanoparticles can be used for both targeted chemotherapy and MRI imaging at the same time as per the research by Singh *et al.* (2020).

## 7.6 Nanotechnology for Overcoming Drug Resistance

Nanocarriers are able to circumvent drug efflux mechanisms by delivering siRNA or CRISPR components to silence resistance-related genes. Thus they provide solutions for multi-drug resistance in breast cancer as per the research by Kumar *et al.*, 2023.

## 7.7 Fusion with AI and ML for Better Results

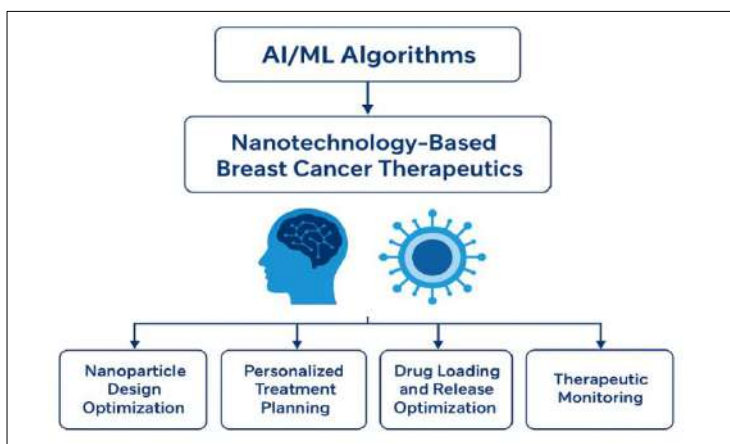
The fusion with AI and ML provides the following results:

- Optimal nanoparticle design parameters can be predicted.
- Drug loading and release kinetics can be modeled.
- Patient-specific treatment strategies can be devised using genomics and imaging data.

This synergy enhances the precision, personalization, and efficiency of nanomedicine in breast cancer care.

## 8. AI/ML Applications in Nano-Based Breast Cancer Therapeutics

The integration of AI and ML with nanotechnology has brought a revolution in the treatment of breast cancer. These technologies provide their benefits in the treatment of breast cancer. AI and ML helps in optimization, prediction, and personalization and nanotechnology helps in the supply of the delivery tools. Fig. 11.3 shows how the fusion of AI and ML with nanotechnology is helpful in the treatment of breast cancer.



**Fig. 11.3** Fusion of AI and ML with Nanotechnology

Various applications of AI and ML in Nano-based breast cancer therapeutics are explained below:

### 8.1 Predictive Modeling of Nanoparticle Properties

AI and ML models are being used frequently to predict the physicochemical characteristics of nanoparticles; these characteristics include size, surface charge, stability, and drug encapsulation efficiency. These predictive abilities help to reduce experimental trial-and-error and enhance the development of optimal nanoformulations (Patel *et al.*, 2021).

Example: To forecast the encapsulation effectiveness and drug release kinetics from PLGA nanoparticles for chemotherapeutic agents; supervised machine learning models such as support vector machines and random forests have been used.

### 8.2 Personalized Treatment Planning

Artificial intelligence (AI) models work on patient-specific multi-omics data including gene expression, proteomics to customize nanomedicine design to individual tumor characteristics. This permits the formation of tailored drug-loaded nanoparticles that relate to the molecular profile of a patient's breast cancer as per the research by Topol (2019) and Zhang *et al.* (2020).

Example: To monitor the surface functionalization of nanoparticles for receptor-targeted delivery and identify molecular subtypes of breast cancer, deep learning models are being used frequently.

### 8.3 Optimization of Drug Loading and Release

AI techniques are being employed to optimize nanoparticle formulation parameters, which thus help to improve drug loading capacity and ensure persistent, precise, or stimuli-responsive release based on tumor microenvironment cues such as pH, enzymes, or redox potential as per the research by Wang *et al.*, 2022.

Example: To dynamically regulate the composition of smart liposomes for real-time adaptation to tumor responses *in vivo*, reinforcement learning is being used.

### 8.4 Nanoparticle Toxicity and Biocompatibility Prediction

Machine learning models help in the evaluation and prediction of nanoparticle toxicity. These models analyze extensive biological response data from *in vitro* and *in vivo* studies. This ensures the safe and efficient development of nanomedicines as per the research by Singh *et al.*, 2020 and Chen *et al.*, 2021.

Example: Neural networks are used to classify nanomaterials as high-risk or low-risk based on structure-activity relationships and experimental toxicity datasets.

### 8.5 Real-Time Tumor Monitoring and Adaptive Therapy

AI-Powered nanosensors are being used in real-time tumor monitoring and adaptive therapy. AI-Powered systems analyze biosensor/nanodevice data to monitor tumor response in real time. These nanosensors then feed this data into ML models to regulate treatment regimens dynamically. These systems result in adaptive dosing and treatment adjustments for better therapeutic outcomes.

Example: ML models with implantable nanosensors are helpful to monitor biomarkers or drug concentrations resulting enhanced outcomes.

### 8.6 Discovery of Novel Nanomaterials and Drugs

AI models are employed to generate novel nanostructures and therapeutic molecules with desired properties. The benefits include designing new ligands, linkers, and surface chemistries for targeted breast cancer treatments according to the study by Zhavoronkov *et al.*, 2019.

Example: To generate candidate nanoparticle formulations with the proposed targeting profiles, Generative adversarial networks (GANs) and variational autoencoders (VAEs) are being utilized.

## 8.7 Imaging and Diagnostic Support

AI algorithms are being utilized for improving the precision of MRI, CT, and fluorescence imaging. The research by Kooi *et al.*, 2017 states that it is beneficial in the detection of tumor margins and monitoring treatment response with increased sensitivity. AI techniques thus enhance the imaging and diagnostic support.

Example: The application of Convolutional Neural Networks (CNNs) in imaging and diagnostic assistance during the treatment of breast cancer.

## 8.8 Drug Resistance Overcoming Strategies

AI tools possess their potential in overcoming drug resistance. They are applicable in detecting resistance markers and optimizing gene-silencing nanoparticle delivery.

Example: Restoring treatment response in drug-resistant tumor types is being performed using ensemble learning and deep learning methods.

Table 11.3 shows various applications of AI and ML in nano-based breast cancer therapeutics together with example technologies and results.

## 9. Advantages of AI and ML in Nano-Based Therapies for Breast Cancer

Artificial intelligence and machine learning with nanotechnology-based methodologies provide revolutionary advantages to the treatment of breast cancer. Such advantages are provided in the research, diagnosis, and therapeutic range. Such technologies find applications in providing more efficient, targeted, and personalized treatments. Some of the advantages are discussed below:

### 9.1 Enhanced Diagnostic Accuracy and Early Detection

AI and ML models are increasingly used for detecting early breast cancer. These models detect molecular data, histopathological images, and mammograms with great accuracy. AI-based tools combined with nano-enabled biosensors and imaging agents can identify tumor markers with greater accuracy, which leads to rapid diagnosis according to the studies by Yala *et al.*, 2019 and Kooi *et al.*, 2017.

### 9.2 Intelligent Design of Nanocarriers

AI and ML technologies assist in nanoparticle design for targeted drug delivery. The models forecast various physicochemical properties like size, surface charge, and composition to deliver the results. For this reason, nanocarrier formation is increased which is beneficial in order to target the tumor tissue and deliver the improved results. This leads to the enhancement in therapeutic potency and decrease in side effects as indicated by the studies of Tiwari *et al.*, 2022 and You *et al.*, 2022.



**Table 11.3** AI/ML Applications in Nano-Based Breast Cancer Therapeutics

Application Area	AI/ML Role	Example Algorithms/ Technologies	Outcome
Nanoparticle Design & Optimization	Predict optimal size, shape, and surface chemistry	Random Forest, SVM	Improved drug delivery and targeting efficiency
Personalized Treatment Planning	Tailor formulations using patient omics and tumor data	Deep Learning, Clustering, XGBoost	Custom therapies for individual tumor profiles
Drug Loading & Release Prediction	Optimize encapsulation efficiency and release kinetics	Regression Models, Reinforcement Learning	Controlled and sustained drug release
Nanotoxicity Assessment	Predict biocompatibility and side effects based on nanoparticle features	Neural Networks, Decision Trees	Safer nanoformulations with reduced systemic toxicity
Therapeutic Monitoring	Analyze biosensor/nanodevice data to monitor tumor response in real-time	Online Learning, Bayesian Models	Adaptive dosing and treatment adjustments
Discovery of Novel Nanomaterials	Generate new therapeutic nanoparticles and drug candidates	GANs, Autoencoders	Accelerated drug discovery with novel nano-bio interfaces
Imaging and Diagnostics	Enhance interpretation of nano-enabled imaging (MRI, CT, optical)	Convolutional Neural Networks (CNNs)	High-sensitivity tumor detection and boundary recognition
Drug Resistance Overcoming Strategies	Identify resistance markers and optimize gene-silencing nanoparticle delivery	Ensemble Learning, Deep Learning	Restoration of treatment response in resistant tumor types

### 9.3 Personalized Treatment Planning

Artificial intelligence (AI) models assist in personalizing nanoparticle-based therapies. They forecast patient-specific genomic, proteomic, and clinical information to deliver the outcomes. Besides, ML models suggest drug combinations, dosages, and release

mechanisms according to the patient-specific tumor profiles which lead to more personalized medicine for breast cancer care according to Topol, 2019 and Zhang *et al.*, 2020.

#### **9.4 Optimized Drug Loading and Controlled Release**

Machine learning models are being used frequently to optimize drug encapsulation efficiency and control release kinetics in nanocarriers. As per the research by Patel *et al.*, 2021 and Patra *et al.*, 2018, it is specifically important for drugs like doxorubicin that are used to treat breast cancer as it improves drug bioavailability, reduces toxicity, and provides persistent therapeutic effects.

#### **9.5 Reduced Experimental Costs and Time**

AI/ML-powered predictive models help to reduce the need for labor-intensive and expensive laboratory experiments. According to the research by Cruz & Wishart, 2006 and Esteva *et al.*, 2019, the virtual screening of nanomaterials and simulation of their interactions with cancer cells simplifies the process of drug development.

AI-driven smart nanodevices integrated with sensors are able to vigorously monitor drug delivery and tumor responses. Also, ML systems are able to analyze sensor data to adjust treatment in real time which results in offering adaptive therapeutic strategies (Singh *et al.*, 2020; Wang *et al.*, 2022).

#### **9.6 Safer and More Effective Treatments**

AI models help in safer and more effective development of nanomedicine. These models help in risk assessment and toxicity prediction for nanoparticles and thus improve the results. As per the research by Chen *et al.*, 2021 and Fadeel *et al.*, 2018, there is increase in the outcomes and decrease in the side effects.

### **10. Challenges and Limitations**

The fusion of (AI), machine learning (ML), and nanotechnology is revolutionizing the breast cancer treatment. But there are some challenges and limitations which hamper the proper implementation. So it is required to address these issues for proper and safe implementation. Different challenges and limitations are explained below:

#### **10.1 Data Quality, Availability, and Integration**

AI and ML models work on huge amounts of high-quality, labeled data which is generated from genomics, imaging, clinical records, and nanoparticle behavior. As per the research by Ching *et al.*, 2018, the data is often fragmented, proprietary, or limited to preclinical studies. Also the integration of such data results in different challenges

which include standardization, interoperability, and computational complexity (Haibe-Kains *et al.*, 2020).

## **10.2 Interpretability and Trust in AI Models**

Many of the ML models act as "black boxes". It means there is only limited insight into how predictions are being made. This issue of interpretability results in lack of trust and acceptance by healthcare providers (Samek *et al.*, 2017). Although Explainable AI (XAI) offers more transparent decisions, it is still in early stage of development in the context of nanomedicine and drug delivery.

## **10.3 Regulatory and Ethical Considerations**

The regulatory and ethical issues are also associated with the use of AI in nanomedicine. Many international bodies including U.S. FDA are still developing systems to assess the safety, efficacy, and accountability of AI-enabled therapeutics (Topol, 2019). Another issues such as algorithmic bias, patient data privacy, and informed consent also become sensitive specifically in the personalized treatment strategies based on the research by Char *et al.*, 2018.

## **10.4 Nanotoxicity and Long-Term Safety Concerns**

Nanotoxicity and long-term safety issues still remain even though nanoparticles offer advantages in targeted drug delivery (Fadeel *et al.*, 2018). Although AI models are able to predict cytotoxicity profiles, but these predictions must be validated rigorously in vivo and clinical testing. Also, it is still difficult for scientists to understand that how nanoparticles interact with biological systems at the molecular level. Table 11.4 shows different challenges and restrictions in AI-ML-Nanotechnology fusion for breast cancer treatment.

There is need to address these issues carefully to utilize the full potential of artificial intelligence and machine learning in nanotechnology based breast cancer therapeutics. There is also need to devise regulatory policies for the safe design of nanoparticles.

## **11. Case Studies**

Artificial intelligence, machine learning and nanotechnology are being extensively used in the treatment of breast cancer. Different case studies have been taken into account to illustrate the usage of these technologies in breast cancer therapeutics. These studies explain how these technologies are being used in improving the treatment and enhancing the patients' outcomes. Table 5 shows different case studies explaining the fusion of AI, ML and nanotechnology to revolutionize the breast cancer treatment.

**Table 11.4** Challenges in AI-ML-Nanotechnology Fusion for Breast Cancer Treatment

Challenge / Limitation	Explanation	Supporting References
Data Quality, Availability, and Integration	AI/ML models require vast, high-quality, and labeled datasets from genomics, imaging, clinical records, and nanoparticle behavior. However, data is often fragmented, proprietary, or restricted to preclinical studies. Integrating diverse datasets faces challenges such as lack of standardization, interoperability issues, and high computational complexity.	Ching <i>et al.</i> , 2018; Haibe-Kains <i>et al.</i> , 2020
Interpretability and Trust in AI Models	Many ML models function as “black boxes” with limited transparency into their decision-making processes. This reduces trust and adoption among healthcare professionals. Explainable AI (XAI) provides more transparency, but it is still in the early stages of application in nanomedicine and drug delivery.	Samek <i>et al.</i> , 2017
Regulatory and Ethical Considerations	Regulatory frameworks for AI-enabled nanomedicine are still evolving. The U.S. FDA and other bodies are working on guidelines for safety, efficacy, and accountability. Ethical concerns include algorithmic bias, patient data privacy, and challenges in informed consent, especially in personalized therapies.	Topol, 2019; Char <i>et al.</i> , 2018
Nanotoxicity and Long-Term Safety Concerns	Although nanoparticles enhance targeted drug delivery, risks of nanotoxicity and long-term safety remain. AI can predict cytotoxicity, but such models require rigorous in vivo and clinical validation. Moreover, understanding nanoparticle interactions with biological systems at the molecular level is still limited.	Fadeel <i>et al.</i> , 2018

**Table 11.5** Case Studies

Case Study	Focus Area	Technology Used	Key Outcome	Reference
AI-Enhanced Nanoparticle Drug Delivery Systems	Optimization of nanoparticle design for drug delivery	ML models, Support Vector Machines (SVM)	Improved prediction of nanoparticle uptake, drug loading efficiency, and release kinetics; reduced experimental workload	You <i>et al.</i> (2022), Patel <i>et al.</i> (2021)
Commercial and Clinical Examples in Breast Cancer Therapeutics	Clinical application of nanomedicine (e.g., Doxil®)	Liposomes, AI/ML for dosing prediction	Doxil® approved for metastatic breast cancer; ongoing AI efforts to improve dosing, predict adverse effects; Nanobiotix and CureMetrix using AI-driven nanomedicine and diagnostics	Barenholz (2012)

Case Study	Focus Area	Technology Used	Key Outcome	Reference
Deep Learning for HER2-Targeted Nanocarrier Design	HER2+ breast cancer targeting with nanoparticles	Deep learning model	40% higher tumor accumulation; reduced off-target toxicity in vivo	You <i>et al.</i> (2022)
AI-Based Prediction of Nanotoxicity	Cytotoxicity prediction of nanocarriers on breast cancer cell lines	Random Forest, SVM	>90% accuracy in predicting toxicity; recommended biocompatible formulations before lab validation	Chen <i>et al.</i> (2021)
Smart Liposomes with Reinforcement Learning	pH-sensitive drug release optimization	Reinforcement Learning (RL)	Improved therapeutic efficacy; reduced cardiotoxicity in TNBC mouse models	Wang <i>et al.</i> (2022)
CNN-Guided Nanosensor Imaging	Early breast cancer diagnosis with nanosensors	CNNs + Quantum dot-based nanosensors	95% sensitivity in early detection; higher specificity vs. conventional immunoassays	Li <i>et al.</i> (2020)
Integrating AI and CRISPR Nanocarriers	Overcoming drug resistance (ER+ breast cancer)	Deep learning + CRISPR/Cas9-loaded nanoparticles	Restored tamoxifen sensitivity; 3-fold higher gene-editing efficiency	Zhang <i>et al.</i> (2021)
Recent Research Studies and Outcomes	Genomic data analysis and smart nanocarriers	Deep learning, RL	30% improved siRNA gene silencing efficiency (Kumar <i>et al.</i> , 2023); RL-controlled pH-sensitive drug release for higher precision (Wang <i>et al.</i> , 2022)	Kumar <i>et al.</i> (2023), Wang <i>et al.</i> (2022)

The use of AI and ML in nanotechnology is bringing a noticeable transformation in breast cancer treatments. As research and development continue to evolve, these innovations are expected to be integrated more widely into oncology workflows, revolutionizing treatment delivery, safety, and personalization.

## 12. Emerging Trends and Future Perspectives

The convergence of artificial intelligence (AI), machine learning (ML), and nanotechnology has brought a significant improvement in based breast cancer therapies. Emerging trends in this context will bring more opportunities in the upcoming years. Different emerging trends and future perspectives are explained blow:

### 12.1 Advances in Explainable AI for Clinical Nanomedicine

As AI adoption increases in healthcare, explainable AI (XAI) is gaining attention to enhance transparency and clinician trust in AI-driven nanotherapeutics (Adadi and

Berrada, 2018). Future systems will likely combine interpretable models with complex deep learning architectures, enabling clinicians to understand and validate predictions related to nanoparticle behavior, drug response, and toxicity; facilitating regulatory approval and clinical adoption.

## **12.2 Combining Real-World Data and Multi-Omics**

Hasin, Seldin, and Lusi (2017) assert that more thorough and dynamic models of the progression of breast cancer and the response to treatment will be possible through the integration of wearable biosensors, real-world clinical data, and multi-omics data (genomics, proteomics, and metabolomics). As patient profiles and tumor microenvironments change, AI/ML algorithms that can integrate these disparate datasets will drive precision nanomedicine designs that adapt to these changes.

## **12.3 Quantum Computing and AI-Driven Nanotechnology Design**

According to Cao *et al.* (2019), quantum computing has the potential to solve intricate optimization issues in drug discovery and nanoparticle design at previously unheard-of speeds. The creation of highly effective and biocompatible nanocarriers for the treatment of breast cancer may be made possible by the future integration of quantum algorithms with AI, which could completely transform the simulation of molecular interactions at the nanoscale.

## **12.4 Smart Nanorobotics and Autonomous Therapeutic Systems**

The research by Kumar *et al.*, 2020, suggests that AI-powered nanorobotics and sensor networks will be capable of facilitating autonomous drug delivery systems that can navigate through the tumor microenvironment, sense cellular conditions, and deliver therapeutics with spatiotemporal precision. These intelligent systems will not only improve effectiveness but also minimize side effects, which are the future systems of personalized breast cancer therapy.

## **12.5 Ethical and Societal Considerations**

Morley *et al.*, 2020 depicts how the future advancement of such technologies needs to be linked with proactive care for ethical and societal issues like data privacy, fairness in algorithms, and equal access to AI-strengthened Nanomedicine. There is need to devise policies to ensure responsible innovation benefiting varied patient populations.

The integration of AI and ML with nanotechnology is a paradigm shift toward more personalized, adaptive, and safe treatments. Along with continued research, clinical validations, and ethical foresights will be essential to realize these promising futures. Table 11.6 shows the emerging trends with their future perspectives.

**Table 11.6** Emerging Trends and Future Perspectives

Emerging Trend	Description	Future Impact	Reference
Explainable AI (XAI) for Clinical Nanomedicine	Use of interpretable AI models to understand predictions on nanoparticle behavior and drug response	Builds clinician trust, improves regulatory compliance, and enhances clinical adoption of AI-driven nanotherapeutics	Adadi & Berrada, 2018
Combining Real-World Data and Multi-Omics	AI/ML models incorporating genomics, proteomics, metabolomics, and real-time data from wearable sensors	Enables dynamic, patient-specific nanomedicine strategies and precision treatment adjustments	Hasin, Seldin, & Lusi, 2017
Quantum Computing in Nanotechnology Design	Combining quantum algorithms with AI for simulating nanoscale molecular interactions	Accelerates discovery of optimized and biocompatible nanocarriers for breast cancer therapy	Cao <i>et al.</i> , 2019
Smart Nanorobotics and Autonomous Systems	AI-powered nanorobots capable of real-time sensing and targeted drug delivery	Delivers therapeutics with high precision, reducing side effects and enhancing personalized treatments	Kumar <i>et al.</i> , 2020
Ethical and Societal Considerations	Addressing privacy, bias, and access in AI-enhanced nanomedicine	Promotes equitable innovation and safeguards patient rights, ensuring responsible deployment	Morley <i>et al.</i> , 2020

## Conclusion

The integration of artificial intelligence and machine learning with nanotechnology is transforming the breast cancer treatment. It has been observed that AI and ML provide powerful tools to analyze biomedical data, enhance nanoparticle design, and personalize treatment strategies, and nanotechnology offers innovative platforms for targeted and controlled drug delivery. These technologies together provide precision medicine techniques to improve therapeutic efficacy, reduce systemic toxicity, and adapt vigorously to patient-specific tumor characteristics. Although significant benefits, challenges of data integration, model interpretability, regulatory frameworks, and ensuring the long-term safety of nanomaterials remain. Overcoming these challenges will require multidisciplinary collaboration, transparency in AI models, and ethical approach to ensure equitable access and patient trust. The emerging trends like explainable AI, integration of multi-omics with real-world data, quantum computing, and smart nanorobotics assure to further revolutionize personalized breast cancer treatment. The combination of AI, ML, and nanotechnology has the potential to be a key component of next-generation oncology treatments as research speeds up and clinical validation increases, ultimately improving the prognosis and quality of life for breast cancer patients around the globe.

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