

Artificial intelligence in cancer therapeutics: Enabling personalized and predictive treatment strategies

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ABSTRACT

Artificial intelligence (AI) is leading the way in revolutionizing precision oncology by allowing cancer treatments to be tailored to individual patient characteristics. The combination of AI with high-throughput sequencing, multi-omics studies, and advanced imaging technologies has paved the way for data-driven models that improve clinical decision making in cancer care. In addition, AI-powered methods have been developed to construct patient-specific tumor growth models, utilizing vast amounts of data to forecast individual treatment responses. These models are designed to customize treatment strategies, thereby enhancing effectiveness while reducing side effects. Importantly, AI has played a crucial role in discovering biomarkers that aid in the early detection of cancer and in predicting how individual patients will respond to different treatments, including chemotherapy, radiotherapy, and immunotherapy. AI-based computational tools support the identification of actionable mutations, optimize radiotherapy planning, and enhance early cancer detection. Despite its significant potential across preclinical and clinical applications, challenges such as data heterogeneity, model interpretability, ethical concerns, and regulatory hurdles remain significant barriers to widespread clinical adoption. By addressing these limitations, AI can further refine individualized cancer treatment, minimizing adverse effects while maximizing therapeutic efficacy. This review comprehensively examines the evolving landscape of AI in precision oncology and highlights future directions to bridge the gap between innovation and clinical application.

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Introduction

The present review mainly focuses on the concept of precision medicine in cancer treatment, the role of Artificial Intelligence (AI) in targeted therapy, drug development, predicting molecular targets, drug repurposing, and the role of AI in precision oncology. Personalized medicine seeks to maximize treatment solutions for individual patients based on their distinct genetic, biochemical, and environmental traits. The availability of large-scale biomedical datasets, advances in high-throughput sequencing technologies, and improvements in computational power drive recent advances in AI. It has proven beneficial for predicting complex protein structures, developing optimized molecular and chemical designs, and discovering new therapeutic targets. AI technologies may reduce costs associated with clinical trials and research by improving efficiency in drug discovery and patient stratification (1, 2). A more precise and targeted approach is replacing the traditional “one-size-fits-all” approach to cancer treatment. The detailed genomic profiling of tumors using innovative technologies such as Next-Generation Sequencing (NGS), Whole Exome Sequencing (WES),

and RNA Sequencing is a pillar of precision oncology. By exploiting these technologies, healthcare professionals can identify specific genetic changes, including mutations, copy number variations, and gene fusions, that contribute to cancer development and influence treatment response (3). Targeted therapies, particularly tyrosine kinase inhibitors and immune checkpoint inhibitors, are administered based on the tumor's molecular profile to target oncogenic pathways and enhance therapeutic efficacy. Liquid biopsies are minimally invasive procedures that identify circulating tumor DNA in blood and have improved the ability to track tumor progression and treatment response in real time (4).

Integrating genomics, transcriptomics, proteomics, metabolomics, and clinical data will deliver a comprehensive understanding of cancer at multiple levels with precision oncology in the future. Breakthroughs in technology, such as big data integration and machine learning, are helping to close the gap towards truly personalized cancer treatment. Although significant progress has been made, several clinical and computational challenges remain. Cancer-related datasets are frequently heterogeneous, high-dimensional, and distributed across various platforms, hindering the

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translation of biological information into actionable therapeutic decisions (5, 6). Also, many current reviews focus on applications in a single field, e.g., cancer diagnosis, radiomics, drug discovery, and/or immunotherapy. They are limited in scope and do not cover the full therapeutic pathway of precision oncology. However, an integrated framework connecting biomarker discovery, therapeutic selection, resistance mechanisms, and treatment monitoring remains limited.

For this purpose, the present review adopts a therapeutics-centric perspective and presents an integrated view of AI-driven precision oncology. Recent developments in the discovery of biomarkers, identification of molecular targets, prediction of drug sensitivity, planning personalized chemotherapy, optimizing radiotherapy, predicting responsiveness to immunotherapy, mechanisms of drug resistance, and oncolytic viral therapy are combined in a single framework. The primary goal of this review is to provide a comprehensive overview of AI's role in precision oncology, with a focus on biomarker discovery, personalized chemotherapy planning, toxicity prediction, radiotherapy optimization, immunotherapy response assessment, drug resistance prediction, targeted drug development, and emerging therapeutic approaches, including oncolytic viral therapy. Furthermore, this review critically examines current issues in data quality, algorithmic bias, interpretability, regulatory considerations, and clinical translation, as well as future research goals that could define the next generation of AI-driven cancer care.

Literature search criteria

This narrative review was developed after conducting a thorough literature search across PubMed, Scopus, Web of Science, and Google Scholar to identify significant publications on the use of AI in cancer therapies. The search was conducted between January and March 2025, focusing on articles published between 2018 and 2025, with seminal studies published before 2018 included where applicable. The search strategy used Boolean combinations of keywords like ("artificial intelligence" OR "machine learning" OR "deep learning") AND ("cancer" OR "oncology"), ("AI" AND "precision oncology"), ("machine learning" AND "immunotherapy"), ("artificial intelligence" AND "drug discovery"), and ("AI" AND "biomarker discovery"). Only authoritative reports, clinical studies, review papers, and peer-reviewed research articles written in English were considered. Excluded were conference abstracts, editorials, letters to the editor, duplicate records, and research unrelated to the use of AI in cancer treatments. Studies addressing biomarker identification, patient stratification, therapy selection, drug discovery, toxicity prediction, resistance monitoring, and clinical translation were selected for inclusion after publications were evaluated for relevance to the title, abstract, and full text. This methodology ensured a thorough and targeted assessment of AI's current role in facilitating tailored and anticipatory cancer treatment approaches.

Conceptual framework of AI-powered precision oncology

AI functions as an integrative platform, connecting many sources of cancer-related data to facilitate personalized therapeutic decision-making. Precision oncology combines data from genetic sequencing, transcriptomics, proteomics,

radiological imaging, digital pathology, and electronic health records to develop a complete patient profile. Machine learning and deep learning algorithms analyze these multimodal datasets to uncover clinically significant patterns, biomarkers, and biological fingerprints associated with disease development and treatment response. In this approach, AI supports numerous interconnected stages of cancer management (7). First, AI helps with biomarker identification and patient classification by finding genetic changes and molecular pathways that influence tumor behavior. Second, AI-assisted radiomics and pathology analysis improve tumor classification and diagnosis accuracy. Third, predictive models use genetic and clinical data to guide treatment decisions, including chemotherapy, targeted therapy, radiation, immunotherapy, and novel treatments such as oncolytic viral therapy (8). Finally, constant monitoring of treatment response and adverse events enables dynamic adaptation of therapeutic strategies, thereby improving clinical outcomes. This integrated framework reveals that AI is more than a collection of individual technologies; it is a comprehensive decision-support ecosystem that enables data-driven precision oncology and tailored cancer treatment (Figure 1).

Machine learning and deep learning in oncology: Genomics, radiomics & clinical data

AI refers to computational systems capable of performing tasks that typically require human intelligence. Machine learning (ML), a subset of AI, allows algorithms to learn patterns from data and improve performance without explicit programming. In contrast, deep learning (DL) uses multilayer neural networks to analyze extremely complex datasets. These technologies have become essential tools in precision oncology, assisting in biomarker discovery, treatment prediction, and tailored cancer management. In the case of bladder cancer, models that improve prognosis for cancer recurrence have been developed using methods such as support vector machines (SVMs), random forests (RFs), artificial neural networks (ANNs), and DL (9, 10). To create comprehensive and complex prediction models, these models use a wide variety of markers, including radiomic, clinical, pathological, and genetic markers (11, 12). Nonetheless, advancements in AI and ML hold considerable promise; there is still much to learn, explore, and validate before these technologies can fully realize their potential in cancer management. Importantly, the machine learning technologies used in bladder cancer are not specific to this disease. Similar methods, such as support vector machines, random forests, ANNs, and deep learning models, have been widely employed in cancer research to evaluate multi-omics, radiomics, and clinical information. Collectively, this research shows how AI approaches can enhance precision oncology by improving patient classification, therapy optimization, and outcome prediction across a wide range of cancer types.

Methodological approaches to machine learning and deep learning models in precision oncology

The performance of AI systems in precision oncology heavily depends on the choice of appropriate ML and DL methods. Different models are intended to manage specific sorts of biomedical data and thus have distinct strengths and limitations.

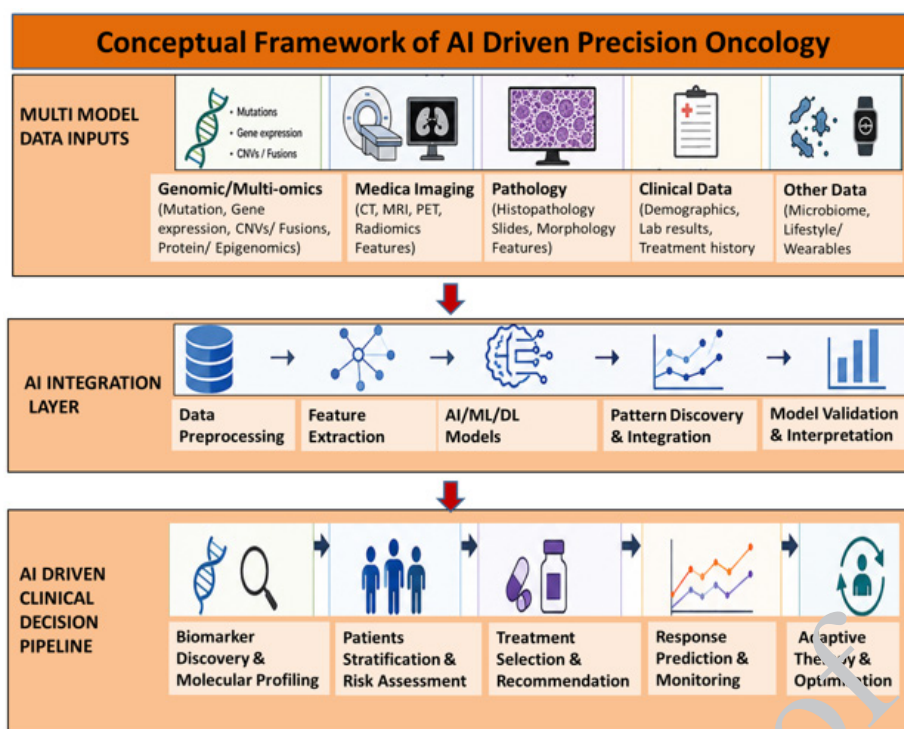


Figure 1. Conceptual framework of AI-driven precision oncology illustrating integration of multi-modal patient data through AI/ML pipelines for biomarker discovery, patient stratification, treatment selection, response prediction, and adaptive therapeutic optimization. AI: Artificial Intelligence, CT: Computed Tomography, MRI: Magnetic Resonance Imaging, PET: Positron Emission Tomography, CNVs: Copy Number Variations

Support Vector Machines (SVMs) are supervised learning methods that classify data by locating the best hyperplane to divide several classes. They are commonly employed in cancer subtype classification and biomarker development, and are especially successful for high-dimensional datasets such as transcriptomic and genomic data. SVMs may model intricate relationships using kernel functions and do well with small training data. However, interpretability remains limited, potentially restricting clinical adoption (13, 14).

Random Forest (RF) algorithms are ensemble machine learning technique called Random Forest (RF) mixes several decision trees to reduce overfitting and increase prediction accuracy. Because it can effectively handle a large number of variables and identify significant predictive features, it is commonly used in genomic, clinical, and multi-omics studies. However, RF models may not adequately capture highly complex nonlinear patterns and can be computationally expensive for very large datasets (15, 16).

Artificial Neural Networks (ANNs) use interconnected computational nodes to process data, like biological neural networks. ANNs have been successfully used to predict therapy response and cancer prognosis because they can represent intricate nonlinear relationships between molecular and clinical factors. However, due to their limited explainability, traditional ANNs are often referred to as “black-box” models and require large amounts of training data (17, 18).

Convolutional Neural Networks (CNNs) are specialized deep learning models frequently used to process medical images. Applications such as tumor identification, image classification, and segmentation are enabled by the automatic extraction of pertinent information from radiology and pathology images. CNNs improve diagnostic accuracy but also require substantial computational power and extensive

annotated datasets, and may perform worse across different imaging platforms or institutions (19, 20).

Deep Learning (DL) models, such as multilayer neural networks and transformer-based architectures, can handle a wide range of data types, including genetic data, radiographic images, pathology reports, and clinical records. They are excellent at detecting complicated biological patterns and enhancing prediction accuracy. However, DL models require large, high-quality datasets and suffer from issues with interpretability, overfitting, reproducibility, and external validation.

Crucially, no single AI model is optimal for all oncology applications. Model selection depends on data type, clinical goals, interpretability needs, and computational resources, with future advances expected to improve reliability and clinical adoption (21-23).

AI model performance in precision oncology is usually assessed using accuracy, sensitivity, specificity, area under the receiver operating characteristic curve (AUC), and concordance index (C-index). Recent studies have demonstrated strong predictive performance across a variety of applications, including digital pathology, radiomics, and multi-omics research. In external validation trials, AI-based pathology models achieved AUCs ranging from 0.746 to 0.999, whereas multimodal clinical decision-support systems commonly reported AUCs of 0.82 to 0.96. Despite these hopeful findings, direct comparison of models is still problematic due to differences in datasets, patient demographics, objectives, and validation methodologies. As a result, rigorous benchmarking, external validation, and prospective clinical studies are critical for ensuring reproducibility, generalizability, and successful clinical translation of AI technologies in precision oncology (24-27).

AI in personalized cancer treatment

AI-driven approaches are tailored for genetic, molecular, and clinical profiles. Genomic analysis is the most effective application of AI (28). AI algorithms are applied to large databases of mutations, gene expressions, and even biomarkers unique to a patient's tumor. Such information would help the doctor select more targeted therapies that are expected to be even more efficacious but less toxic than traditional treatments (29). AI-empowered imaging thereby enables machine-learning algorithms to analyze CT, MRI, and PET scans from individual patients more thoroughly. This results in earlier tumor identification, which may facilitate much earlier personalized treatment planning (30). AI-driven chatbots and Virtual health assistants provide personalized patient guidance throughout treatment, including treatment plans, medication schedules, and possible side effects (31). However, AI has enhanced the precision, personalization, and efficacy of cancer treatment, improving patient outcomes while making therapies more targeted for each individual. This change will transform the oncology landscape into one that is data-powered and grounded in therapeutic strategies.

AI-based drug sensitivity prediction

The primary area of progress is in ML and DL algorithms for predicting individual tumor drug responses to various chemotherapeutic agents. Although traditional oncology employs treatment based on general protocols, AI systems can handle massive, multidimensional datasets, including genomic, proteomic, and transcriptomic data, to discover specific biomarkers associated with drug sensitivity or resistance in a patient (32). Such biomarkers guide the oncologist in selecting specific therapies most effective for an individual, rather than relying on trial and error or best-guess methods. Such a model could be DeepDSC, which utilizes DL approaches to evaluate gene expression profiles and predict drug efficacy across various cancer types. This model enhances prediction accuracy and adapts to new data inputs (33).

Personalized chemotherapy planning

Moreover, patient tumor organoids (miniaturized, three-dimensional tumor models grown from autologous or self-derived cells) are used alongside AI algorithms to test drug sensitivity *in vitro* (32). AI-driven simulations are fed comprehensive databases, such as the Genomics of Drug Sensitivity in Cancer and the Cancer Cell Line Encyclopedia, which include thousands of annotated drug-tumor interaction records (34). Regular retraining of these models using current clinical outcomes leads to continuous improvements in predictive accuracy. AI provides access to an entirely new dimension in personalized chemotherapy. It compiles all aspects of an individual's health record, including Electronic Health Records, genetic test results, imaging data, and clinical histories. AI tools can individualize treatment plans for specific patients (35). These algorithms will consider everything from tumor histology and molecular subtypes to organ function, prior treatment responses, and occasionally patient preferences. While AI-guided chemotherapy planning seeks to determine the most effective treatment regimen, providing optimal cancer care also necessitates reducing treatment-related toxicity. Due to interpatient variability in drug metabolism and tolerance,

AI models are increasingly being utilized to forecast adverse events and toxicity risks. This dual capability enables a more comprehensive precision oncology strategy by maximizing both therapy efficacy and patient safety.

Toxicity and side effect prediction

AI plays a significant role in enhancing the safety of chemotherapy treatment by predicting potential toxicities in individual patients before treatment begins. From pharmacogenomics, lab tests, and comorbidity profiles, ML models would predict risks such as neutropenia (low white blood cell count), cardiotoxicity, hepatotoxicity, and gastrointestinal complications (36). A model will indicate if a patient with specific genetic variants would be at higher risk for anthracycline-induced heart damage or liver issues from particular targeted therapies. These tools would enable the clinician to adjust dosages or switch to alternative agents, thereby minimizing the chances of serious complications (28). Additionally, AI systems can monitor patients undergoing treatment in real time by tracking side-effect profiles, lab results, and symptoms reported throughout chemotherapy (37). Beyond enhancing systemic therapies like chemotherapy, AI is also revolutionizing locoregional cancer treatments. AI can evaluate imaging and clinical data to increase the accuracy, efficiency, and personalization of radiation planning, just as it does in predicting treatment response and toxicity. These developments demonstrate how AI contributes to numerous therapeutic modalities within the precision oncology paradigm.

AI-guided radiotherapy planning

Radiotherapy is a cornerstone of cancer treatment, used in more than half of all cancer patients worldwide. Successful therapy with radiotherapy requires thorough planning. This involves three primary steps: locating both the tumor and surrounding healthy tissues, determining the appropriate radiation dose, and aligning the beams to maximize effectiveness while minimizing unwanted effects (38). This process is time-intensive and requires multidisciplinary collaboration among radiation oncologists, dosimetrists, and physicists. Planning can take hours per patient and often varies because individuals interpret images differently. AI, through ML and DL, has brought significant progress in radiotherapy planning (39). It reduces planning time and improves consistency and precision. Although radiotherapy remains a cornerstone of cancer treatment, the increasing importance of immunotherapy has opened up new avenues for AI-driven predictive modeling. As response rates to immune checkpoint inhibitors vary widely among patients, AI is increasingly used to identify biomarkers and predict treatment outcomes, enabling more precise patient selection and treatment optimization.

AI in image segmentation

AI's first significant role in radiotherapy lies in image auto-segmentation. To deliver precise radiotherapy without damaging nearby sensitive structures, accurate maps of tumors and organs at risk are essential (40). Using large training datasets and deep CNNs, this process achieves precision equal to, or sometimes surpassing, that of human specialists. A landmark study by Back D.A. in 2020, conducted in collaboration with DeepMind and the UK National Health Service, demonstrated that a DL system

can automatically segment 21 head and neck organs at risk on CT scans with clinical-level accuracy, achieving Dice similarity coefficients greater than 90% for most structures. Such systems can reduce contouring time by up to 76%, enabling faster treatment initiation (38).

Clinical deployment of AI segmentation tools

Clinical products such as Limbus AI, MVision AI, and Mirada RTx are now integrated into clinical workflows worldwide. Such AI automation is especially valuable in high-throughput settings and regions with limited access to experienced personnel. Aside from segmentation, AI is increasingly used for plan generation and dose prediction.

Dose prediction and plan generation

Traditional dose planning involves iterative trial-and-error optimization by the dosimetrist, often based on institutional knowledge. In contrast, AI models can learn from large databases of historical treatment plans to predict the best-suited 3D dose distributions for new cases. This study developed a DL model capable of accurately predicting clinically acceptable dose distributions for prostate intensity-modulated radiotherapy from patient anatomy input. It matched quantitatively with manually planned cases, but in significantly less time (39-43).

Beam configuration and optimization

Optimization, the other vital phase of radiotherapy planning, has also been transformed using AI. Reinforcement learning techniques enable AI agents to experiment with various beam configurations and evaluate the quality of generated plans using reward functions that reflect dosimetric specifications. A deep reinforcement learning technique for treatment planning of non-small cell lung cancer was discussed (44). Comprehensive platforms such as Varian Ethos and RaySearch's RayStation with RayIntelligence, enable the practical integration of AI into clinical workflows. These platforms offer end-to-end AI planning capabilities, including automated contouring, dose prediction, and adaptive re-planning (45). One clinical example from the implementation of the Varian Ethos platform was a 55-year-old patient who received a 15% dose reduction to the optic apparatus compared to the reference plan. The plan required only minor adjustments and was signed off by the planning team in under 30 min (National Cancer Institute, 2024)(46). Besides improving efficiency, AI also supports greater consistency between patients and planners. Such consistency is crucial in multi-institution trials and collaborative oncology networks. AI can also help ensure equitable access to quality radiotherapy in low- and middle-income countries with limited human resources and expertise. By reducing dependence on specialist availability, AI democratizes precision oncology by granting access irrespective of availability (45). However, despite these promising developments, several challenges remain. AI models are highly dependent on the quality and variety of training data. Models trained on a biased or narrow dataset may fail to generalize to different populations or imaging protocols (47). Clinicians can only use an AI system for decision-making if they understand how and why it makes its recommendations (48).

Immunotherapy response prediction

Typically, the immune response determines whether

a treatment is successful. Such treatments include immunotherapy and vaccinations. Immune responses in individuals are influenced by genetics, age, gut microbiota, and comorbidity (49). Using predictive modeling allows doctors to group patients by expected outcomes, making treatments more effective and safer (50). AI also helps identify biomarkers and molecular signatures that indicate a patient's potential response to specific therapies. Thus, the era of one-size-fits-all approaches to medicine is past, ushering in individualized, precision-medicine treatment methods (51).

Cancer immunotherapy uses immune response prediction and has demonstrated significant potential. As a potent tool, AI aids in assessing patient responses to treatment with immune checkpoint inhibitors, such as PD-1 and PD-L1 blockade therapies (52). It evaluates treatment outcomes based on genetic alterations, tumor microenvironment characteristics, and T-cell receptor repertoires (53). Developing personalized cancer vaccines is another application of AI. This improves the effectiveness of the treatment and reduces unwanted side effects. The potential of AI to anticipate therapeutic responses extends beyond immunotherapy and provides useful insights for developing targeted treatment methods. By combining genomic, transcriptomic, and proteomic data, AI can uncover actionable molecular changes and aid in the development of novel therapeutic targets, ultimately advancing the next generation of precision cancer therapies.

Targeted therapy development

Targeted treatments focus on adjusting specific molecular pathways linked to disease progression. This approach enables precise treatments that minimize unwanted side effects. AI enhances this process by analyzing data from various biological layers, including genomics, proteomics, and transcriptomics, to identify potential treatment targets (54). By processing this information, AI enhances the accuracy of targeting decisions. AI also uses ML to explore complicated biological networks. These models spot patterns and help predict which proteins or genes can be targeted in treatment. An example is the use of AI tools to identify new anticancer targets (55). By mapping how cells interact within biological networks associated with diseases such as cancer, these tools aid in identifying new targets and developing novel medicines (56).

Drug discovery

Drug discovery has traditionally been a time-consuming, expensive, and high-risk procedure. Recent breakthroughs in AI have sped target discovery, virtual screening, and lead optimization, increasing the efficiency of drug development (57,58). A notable example is halicin, a novel type of antibiotic discovered using DL software developed by researchers at the Massachusetts Institute of Technology. Although halicin was identified in the context of antimicrobial drug discovery, this example demonstrates AI algorithms' ability to efficiently screen large chemical libraries, predict biological activity, and prioritize promising therapeutic candidates. Similar AI-driven approaches are increasingly being applied in oncology to identify novel anticancer agents, optimize targeted therapies, and accelerate precision drug development. The AI system reviewed more than 100 million molecules and identified one that is effective

against a wide range of harmful microbes, including those resistant to conventional antibiotics (59, 60). AI helps create small-molecule inhibitors that target specific proteins linked to diseases. Scientists utilized AI tools to identify a new inhibitor for Cyclin-dependent Kinase 20 (CDK20), a protein associated with cancer growth (Figure 2).

Predicting molecular targets and resistance mechanisms

AI has sparked a revolution in biomedical research, particularly in the fields of drug discovery and development. AI leverages large datasets and advanced algorithms to identify molecular targets and understand resistance mechanisms. This enhances the precision and effectiveness of therapies. Identifying valid molecular targets is crucial for developing new and effective drugs. AI accelerates this process by analyzing various layers of data, including genomics, proteomics, and transcriptomics. It investigates these datasets to spot potential treatment options. Using ML, patterns in complex biological systems are identified, and genes or proteins that could serve as targets for treating illnesses are determined (61).

Predict resistance mechanisms

Dealing with drug resistance is one of the biggest challenges in treating diseases like cancer and infections. AI has a vital role in helping scientists predict how resistance develops. It achieves this by analyzing genetic and physical data to identify patterns associated with resistance. ML models now help predict how cancer cells resist chemotherapy. One study applied algorithms such as Naïve Bayes, K-Nearest Neighbors, Decision Trees, Random Forests, and Neural Networks to categorize cancer cell lines into groups that respond to or resist Cisplatin. This study highlighted the importance of genes such as PTEN3 and CTNNB1 in contributing to resistance (62, 63). AI-based resistance prediction models are highly relevant in oncology, even outside infectious disorders. Machine learning algorithms can detect molecular signatures associated with chemotherapy resistance, targeted therapy resistance,

and immunotherapy failure by integrating genomic, transcriptomic, and clinical data. In precision oncology, these prediction methods could support early therapeutic intervention and individualized treatment planning. This helps researchers track and understand how resistance develops (64-66). Additionally, teamwork between AI professionals and biology experts is crucial to ensuring that these models are both precise and meaningful in real-world biological applications (67, 68). AI tools, when combined, enable scientists to identify and confirm new treatment targets. This accelerates the process of developing more effective medicines (69). Collectively, these studies illustrate AI's growing importance in understanding and predicting treatment resistance, one of the most significant hurdles to effective cancer therapy. AI's capacity to detect resistance-associated biomarkers and biological pathways may aid patient assessment, therapy selection, and the development of more effective, tailored therapeutic regimens (Figure 3).

Biological and clinical interpretation of AI predictions in precision oncology

Beyond enhancing forecast accuracy, AI is crucial for extracting physiologically meaningful insights from complex cancer datasets. By combining genomic, transcriptomic, proteomic, radiomic, and clinical data, AI can identify molecular patterns that enhance understanding of tumor biology and therapeutic decision-making (70). Characterizing tumor heterogeneity is one of the most important uses of AI. AI can detect distinct genetic subgroups within cancers using multi-omics data, highlighting differences in disease progression, metastatic potential, and therapy sensitivity. This information allows for more precise patient classification and individualized treatment plans. AI also helps in understanding the processes underlying medication resistance. Machine learning algorithms can identify genetic changes, signaling networks, and gene expression patterns associated with resistance to chemotherapy, targeted treatments, and immunotherapies (71-73). These findings may aid in

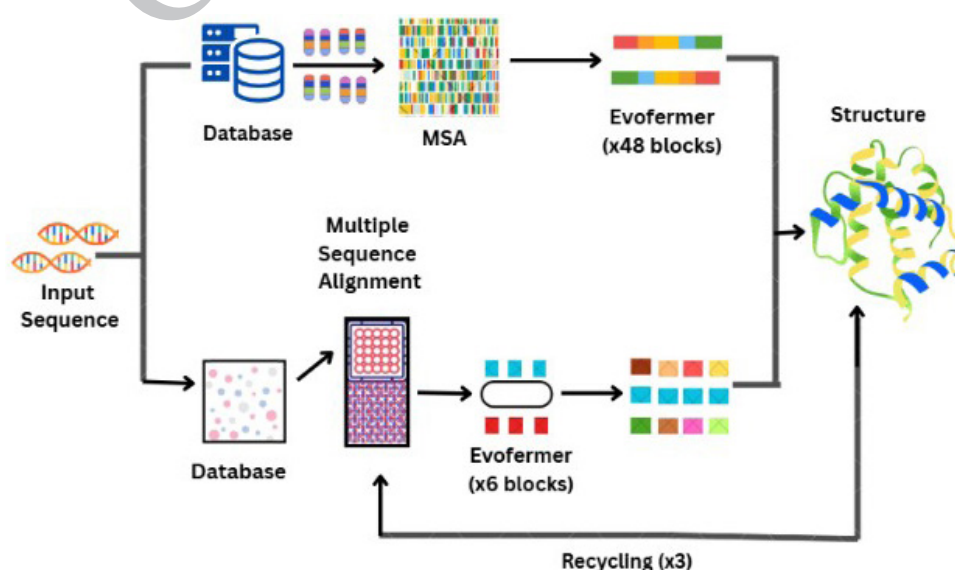


Figure 2. AI-assisted protein structure prediction for precision drug discovery

The Evoformer-based approach accurately predicts three-dimensional protein structures from sequence data, making it easier to identify targets, analyze molecular interactions, create rational drugs, and speed the development of customized anticancer medicines
MSA: Multiple Sequence Alignment

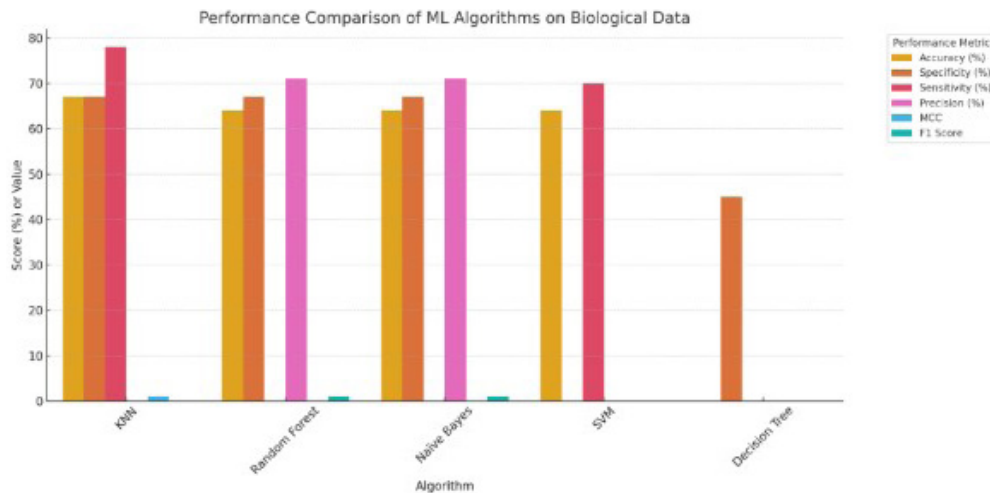


Figure 3. Conceptual comparison of traditional machine learning algorithms used in precision oncology, including SVM, RF, DT, NB, and ANN

The figure summarizes their characteristics, strengths, limitations, interpretability, and applications in cancer research. It is intended for educational purposes and not as a performance benchmark. Deep learning methods are discussed separately due to their distinct architectures and applications

SVM: Support vector machine; RF: Random forests; DT: Decision Tree; NB: Naïve Bayes; ANN: Artificial neural network; ML: Machine learning; KNN: K-Nearest Neighbors; MCC: Matthews Correlation Coefficient, F1: F1 Score / F1 Measure

identifying new therapeutic targets and developing more effective combination treatments. Furthermore, AI enhances patient stratification by categorizing patients based on genetic and phenotypic variables rather than traditional histological markers alone. This method simplifies the identification of patients who are most likely to benefit from specific therapies. As a result, AI goes beyond prediction by connecting computer outputs to biological pathways, increasing our grasp of cancer complexity and enabling more precise, tailored oncology care (74, 75)

AI applications in precision oncology are increasingly expanding into new therapeutics, such as oncolytic viral therapy (OVT). AI aids in patient selection, response prediction, and treatment optimization by combining multimodal genetic, immunological, and clinical data. Thus, OVT is a natural extension of the larger AI-driven precision oncology paradigm. One such example is oncolytic viral therapy, where AI integrates genetic, immunological, and clinical data to optimize patient selection and treatment design.

Personalized oncolytic viral therapy

Oncolytic viral therapy (OVT) is a new component of precision oncology that uses genetically produced or naturally occurring viruses to precisely attack and destroy tumor cells while also activating anti-tumor immune responses. OVT efficiency is determined by a variety of biological parameters, including tumor genetic features, the composition of the immunological microenvironment, viral tropism, and the host immune response. Because these characteristics yield complex statistical patterns, AI has emerged as a viable tool for optimizing patient selection, predicting therapy efficacy, identifying predictive biomarkers, and developing tailored treatment regimens. Thus, OVT is an excellent example of how AI might help translate biological complexity into individualized cancer treatment (Figure 4)(76-80).

Predicting tumor and virus interaction

Understanding the way tumors, viruses, and the immune system interact makes it tough to predict how treatments

will work. Researchers have built AI models to simulate these interactions and improve OVT treatment plans (81). A good example is a hybrid ecological model. It combines time-delayed Generalized Lotka-Volterra equations with optimization tools, such as Genetic Algorithms and Reinforcement Learning. This setup has proven highly accurate at predicting how OVT works. The model highlighted key biomarkers, including TNF, NF- κ B, and IL-18, that play crucial roles in monitoring tumor growth and treatment effectiveness (82).

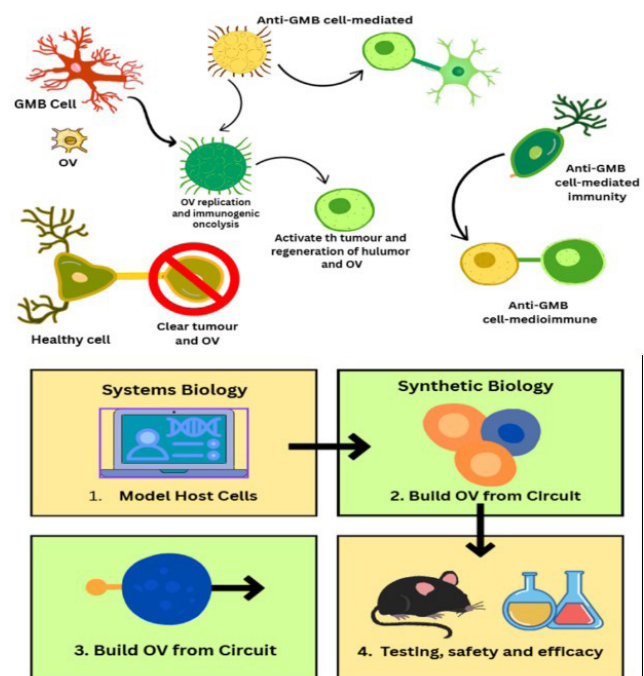


Figure 4. AI-enabled development of personalized oncolytic viral therapy, illustrating how systems biology, synthetic biology, and AI support biomarker discovery, prediction of tumor–virus interactions, viral engineering optimization, and individualized treatment design for glioblastoma and other cancers

GBM: Glioblastoma multiforme, OV: Oncolytic virus, Anti-GBM: Anti-glioblastoma multiforme

Neoantigen identification and vaccine design

Cancer vaccines tailored to target tumor-specific neoantigens have become a key component of immunotherapy. AI enhances chemotherapy safety by enabling early prediction of treatment-related toxicities (83). ML tools such as EasyFuse help identify cancer-associated gene fusions that can generate immunogenic neoantigens. Companies like Transgene collaborate with NEC Corporation to utilize AI-powered tools to select neoantigens, thereby helping to design custom cancer vaccines that enhance the precision and effectiveness of immunotherapy.

Talimogene Laherparepvec (T-VEC): T-VEC is a modified herpes simplex virus type 1 and stands as the first oncolytic virus approved by the FDA to treat melanoma. It is designed to produce GM-CSF and multiply inside tumors. This process leads to cell destruction and triggers a widespread immune response against the tumor (84, 30). Teseptarev (G47Δ): Teseptarev, or G47Δ, is an oncolytic herpes simplex virus used in Japan to treat malignant glioma. Research from clinical studies shows that patients with recurrent or residual glioblastoma had a one-year survival rate of 84.2%. The median overall life expectancy reached 20.2 months (30). Pelareorep, an unaltered human reovirus, is being studied for its ability to promote an inflammatory tumor microenvironment and attack cancers. Early trials suggest that it might work against cancers such as breast, colorectal, and pancreatic types (85). Overall, these data show that AI improves OVT not only through enhanced predictive skills, but also by enhancing our understanding of tumor-virus-immune relationships. By combining genomic, immunological, and clinical data, AI can identify patients who are most likely to benefit from viral therapies, anticipate resistance mechanisms, and enhance individualized treatment plans. Thus, OVT represents AI's broader role in precision oncology, in which computational tools convert complex biological data into clinically actionable treatment ideas (86-88). Table 1 summarizes representative AI-based approaches used in cancers for prognosis, mutation prediction, and treatment response assessment (89-113).

Integrative role of AI in precision oncology

AI has the potential to impact every step of the precision oncology pipeline by integrating diverse biological and clinical data to provide more actionable insights into therapies. Multi-Omics data, such as genomic, transcriptomic, proteomic, and epigenomic profiles, enable the identification of molecular changes and therapeutic targets, while radiomics and medical imaging provide non-invasive characterization of the tumor phenotype and therapeutic response. The combination of these heterogeneous datasets and clinical parameters with machine learning and deep learning models enables biomarker discovery, stratification, treatment selection, prediction of treatment response, and monitoring for treatment resistance. AI is not just a standalone analytical tool; it is a cohesive platform that integrates data generation, biological interpretation, and clinical decision-making, paving the way for personalized and adaptive cancer treatment (114-116).

Apart from these developments in AI in oncology, there is no one-size-fits-all optimal AI solution for precision

oncology applications. In contrast, conventional machine learning algorithms such as Support Vector Machines, Random Forests, and Logistic Regression remain useful for structured clinical and genomic data due to their relatively low computational demand and interpretability. In contrast, deep learning models have shown great potential to extract complex patterns from radiological images, histopathology slides, and multi-omics data, leading to improved predictability in diagnostics, prognosis, and treatment responses in these areas. Improved predictive accuracy, however, can come at the cost of interpretability, posing a challenge to the uptake of the models in clinical practice. Additionally, differences in patient samples, data quality, sample sizes, feature selection methods, and validation protocols across studies contribute to variability in AI model performance. The future of precision oncology may be a combination of multi-modal frameworks that integrate biological, imaging, and clinical information rather than relying on a single AI model, and that are transparent, robust, and clinically useful (117-120). AI serves as an integrated platform along the precision oncology continuum. AI-powered analysis of multi-omics, radiological, pathological, and clinical data identifies diagnostic and prognostic biomarkers, aids patient classification, and promotes personalized treatment selection. Furthermore, machine learning models can predict treatment outcomes, assess toxicity risks, and identify mechanisms of therapeutic resistance. Continuous integration of longitudinal patient data enables dynamic monitoring of illness development and treatment outcomes, facilitating adaptive clinical decision-making. These integrated applications offer AI as a unified foundation for modern cancer care, linking biomarker discovery, therapeutic optimization, resistance monitoring, and clinical translation.

Challenges, limitations, and clinical translation of AI in precision oncology

Despite encouraging improvements, several hurdles prevent the routine use of AI in precision oncology. One key limitation is data heterogeneity, which arises when datasets are generated across diverse platforms, methods, and patient populations, undermining model consistency and reproducibility. Another problem is algorithmic bias, which occurs when training data does not adequately represent diverse groups, leading to unequal therapeutic outcomes. A lack of external validation also reduces clinical confidence. Many AI models perform well in retrospective studies but fail to replicate these outcomes in independent patient cohorts. Furthermore, the complexity of many machine learning and deep learning models limits interpretability, making it challenging for clinicians to understand and trust AI predictions. Other impediments include legal restrictions, data privacy and security concerns, interoperability issues, and integration with existing healthcare systems. Addressing these technical, ethical, and operational concerns requires thorough validation and multidisciplinary teamwork to ensure successful clinical translation. AI clinical translation in precision cancer entails overcoming hurdles such as data quality, heterogeneity, model interpretability, privacy, and regulatory approval. Many AI systems are built using retrospective datasets, which limits their applicability across patient groups. Furthermore, the "black-box" nature of complicated algorithms can erode clinical trust and

Table 1. Artificial intelligence (AI) and Machine learning (ML) models for cancer use multi-omics and radiomics data to predict prognosis, mutation status, treatment response, and tailored cancer therapy

Cancer Type	AI methods/algorithm	Inputs	Validation Status	Dataset size	Clinical outcome	Major Limitations	References
Breast cancer	ConcatAE and CrossAE	Multiomics	Internal validation	Moderate-sized cohort	Risk stratification and prognosis prediction	Limited external validation; potential overfitting	(89)
Breast cancer	Naïve Bayes classifier, random forest, SVM with polynomial kernel, and SVM with RBF kernel	Proteomics	Internal validation	Small-to-moderate cohort	Molecular classification and prognosis assessment	Limited generalizability; proteomic variability	(90)
Breast cancer	XGBoost (eXtreme Gradient Boosting)	Transcriptomics	Internal validation	Moderate-sized cohort	Prognostic categorization and treatment guidance	Requires validation in independent populations	(91)
Breast cancer	DT (decision trees)	Genomics	Internal validation	Large imaging dataset	Histopathological classification and prognosis	Black-box interpretation; computationally intensive	(92)
Breast cancer	VGG16, VGG19, and ResNet50 and SVM	Genomics	Internal validation	Large imaging dataset	Histopathological classification and prognosis	Black-box interpretation; computationally intensive	(92)
Breast cancer	Classification and regression tree (CART), Naïve Bayes (NB), and SVM	Radiomic	Internal validation	Moderate-sized imaging cohort	Prediction of chemotherapy response	Single-center dataset; radiomic feature variability	(93)
Rectal Cancer	Logistic regression (LR), DT, and SVM	Radiomics	Internal validation	Moderate-sized imaging cohort	KRAS mutation prediction for targeted therapy selection	Limited multicenter validation	(94)
Locally advanced rectal cancer (LARC)	SVM, Bayesian model, ensemble learning methods, and logistic regression	Radiomics	Internal and external validation	Moderate-sized cohort	Personalized chemoradiotherapy planning	Model performance influenced by imaging protocols	(95)
(LARC)	CFs-SVM	Genomics	Internal validation	Small-to-moderate cohort	Prediction of neoadjuvant treatment response	Requires prospective validation	(96)
LARC	DT	Radiomics	Internal validation	Moderate-sized MRI dataset	Prediction of pCR, TRG, and NAR score	Moderate predictive accuracy; limited generalizability	(97)
Colorectal cancer (CRC)	DT	Radiomics	Internal validation	Moderate-sized imaging cohort	FOLFOX response prediction	Retrospective design; limited external validation	(98)
CRC	LASSO	Genomics	Internal validation	Large genomic cohort	Prediction of lymph node metastasis	Population-specific genomic signatures	(99)
CRC	Random forest (RF), DT	Genomics	Internal validation	Moderate-to-large genomic cohort	Personalized treatment and TNM staging	Requires prospective clinical assessment	(100)
CRC	LASSO regression and stepwise Cox	Genomics and bioinformatics	Internal and external validation	Large cohort (>2500 patients)	Risk stratification and surveillance optimization	Biological interpretation of lncRNA signatures remains challenging	(101)
CRC	Artificial neural network method (ANN)	Radiomics	Internal validation	Moderate-sized imaging cohort	RAS, BRAF mutation prediction and patient stratification	Limited interpretability of ANN models	(102)
CRC	Gaussian naïve Bayesian classifier	Radiomics	Internal validation	Small HER2-positive cohort	Prediction of targeted therapy response	Small sample size; restricted applicability	(103)
Oral cancer	Convolutional Neural Networks (CNNs) and Vision Transformers (ViTs)	Genomics and bioinformatics	Internal validation	Large multi-omic datasets	Personalized treatment planning	High computational demands; need for external validation	(104)
Oral cancer	Mesmer	Genomics	Internal validation	Moderate-sized cohort	Biomarker discovery and recurrence risk assessment	Requires validation across diverse populations	(105)
Gastric cancer	CNN (ResNet50)	Genomics	Internal validation	Large imaging dataset	Metastasis prediction and staging	Performance dependent on image quality	(106)
Gastric cancer	CNN-CAD ResNet50	Radiomics	Internal and external validation	Large endoscopic image dataset	Invasion depth assessment and preoperative planning	Generalizability across imaging systems remains uncertain	(107)
Gastric cancer	Bidirectional deep neural networks	Transcriptomics and genomics	Internal validation	Moderate-sized multi-omics cohort	Survival stratification	Limited interpretability of deep neural networks	(108)
Gastrointestinal cancers	ML/DL model	Genomics	Multiple validation approaches reported	Multiple datasets	Broad support for personalized oncology	Heterogeneity among included studies	(109)
Gastrointestinal cancer	Genomic mutation signature (GMS)	Genomics	Internal validation	Large genomic cohort	Prediction of immunotherapy benefit	Requires prospective clinical validation	(110)
Ovarian cancer	DL	Multi-omics	Internal validation	Moderate-sized multi-omics dataset	Molecular subtype identification	Limited external validation	(111)
Acute myeloid leukemia	Drug Ranking Using ML	Multi-omics	Internal validation	Multi-cohort dataset	Drug prioritization and therapy selection	Prospective clinical utility remains to be established	(112)
Liver, breast and pancreatic cancer	DeepProg	Multi-omics	Internal and external validation	Large multi-omics datasets	Survival-risk prediction across cancers	Complexity and limited biological interpretability	(113)

AE: autoencoder; ConcatAE: concatenated autoencoder; CrossAE: Cross-modal/cross-domain autoencoder; XGBoost: eXtreme Gradient Boosting; DT: decision tree; SVM: support vector machine; RBF: radial basis function; CART: classification and regression tree; NB: naïve Bayes; LR: logistic regression; LARC: locally advanced rectal cancer; CFs-SVM: CFS-based support vector machine; MRI: magnetic resonance imaging; pCR: pathological complete response; TRG: tumor regression grade; NAR: neoadjuvant rectal score; CRC: colorectal cancer; FOLFOX: folinic acid, fluorouracil, and oxaliplatin; LASSO: least absolute shrinkage and selection operator; RF: random forest; TNM: tumor, node, and metastasis; ANN: artificial neural network; RAS: rat sarcoma; BRAF: B-Raf proto-oncogene; HER2: human epidermal growth factor receptor 2; CNN: convolutional neural network; ViT: vision transformer; CAD: computer-aided diagnosis; CNN-CAD: convolutional neural network–computer-aided diagnosis; ML: machine learning; DL: deep learning; ML/DL: machine learning/deep learning; GMS: genomic mutation signature; and KRAS: Kirsten rat sarcoma virus

acceptance. Prospective multicenter validation studies are required to ensure reliability, safety, and clinical value. Explainable AI, consistent data frameworks, and seamless integration into clinical processes will be critical to transforming AI-driven discoveries into routine practice and advancing individualized cancer therapy.

Conclusion and future perspectives

AI is poised to transform precision oncology by enabling the integration of multimodal biological and clinical data to improve diagnosis, prognosis, and therapeutic decision-making. While machine learning and deep learning models have excelled in cancer research, their clinical application is hampered by data quality, interpretability, and validation issues. Multimodal AI frameworks, explainable models, federated learning, and thorough clinical validation will be critical to future advancement. AI has the potential to deliver completely personalized, adaptive cancer therapy as it advances.

Future breakthroughs in precision oncology will increasingly depend on multimodal frameworks that integrate genomic, transcriptomic, proteomic, radiomic, and clinical data. To achieve wider clinical adoption, explainable and trustworthy AI systems, federated learning approaches, and future clinical validation studies will all be key to success. AI is a powerful catalyst in revolutionizing precision oncology by enabling the integration and analysis of complex clinical, imaging, and genetic data. It helps with more precise prognostication, earlier diagnosis, and personalized treatment strategies tailored to each patient's cancer profile. Eventually, these advances will support real-time therapeutic decisions and enable truly personalized cancer treatment. In the future, AI will become an important tool in oncology, with ongoing, more intensive study, verification, and ethical guidance. However, various obstacles still impede AI-based treatment, including data quality, algorithmic transparency, ethical issues, regulatory approval, and health equity.

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Authors' Contributions

S R was responsible for the study's conception, design, drafting, and approval of the final version of the manuscript; N F conducted the literature search, drafted the manuscript, and reviewed it; N H wrote the manuscript; T B conducted the literature search and prepared the draft; A Z wrote the manuscript and reviewed it; ST R supervised and reviewed, and approved the final version of the manuscript; F M supervised and reviewed, and approved the final version of the manuscript. After reading the manuscript, all authors approved its publication.

Conflicts of Interest

No conflict of interest to declare.

Declaration

The manuscript has been read and approved by all the authors. This manuscript was created using generative AI methods. Specifically, the most recent version of OpenAI's ChatGPT was used to improve language, edit content, and generate summaries.

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