

Foundation AI Models for Predictive Cancer Therapeutics: From Biomarker Discovery to Clinical Translation

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ABSTRACT:

The rapid evolution of artificial intelligence (AI) has fundamentally transformed precision oncology by enabling predictive computational models that integrate heterogeneous biomedical data for individualized therapeutic decision-making. Among recent technological advances, foundation AI models have emerged as powerful computational frameworks capable of learning generalized biomedical representations from large-scale multimodal datasets and subsequently adapting to numerous downstream oncology applications. Unlike conventional machine learning algorithms trained for isolated predictive tasks, foundation models leverage self-supervised learning, transformer architectures, multimodal representation learning, graph neural networks, and generative AI to integrate radiological imaging, digital pathology, genomics, transcriptomics, proteomics, metabolomics, spatial biology, laboratory biomarkers, electronic health records, and longitudinal clinical outcomes into unified patient-centered computational representations. These intelligent systems are revolutionizing biomarker discovery, therapeutic response prediction, drug target identification, immunotherapy optimization, adaptive treatment planning, digital twins, and clinical decision support while accelerating translational oncology research. Recent developments in large language models, retrieval-augmented generation, reinforcement learning, federated learning, agentic AI, and explainable artificial intelligence have further expanded the capabilities of predictive cancer therapeutics. Despite remarkable progress, significant challenges remain regarding multimodal data harmonization, computational scalability, interpretability, interoperability, regulatory validation, ethical governance, and equitable implementation. This review provides a comprehensive overview of foundation AI models for predictive cancer therapeutics, emphasizing computational principles, biomarker discovery, clinical applications, translational challenges, and future perspectives for advancing precision oncology.[1]

Keyword: Foundation models, Artificial intelligence, Predictive therapeutics, Precision oncology, Biomarker discovery, Multi-omics, Digital pathology, Clinical translation, Personalized medicine, Computational oncology.

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1.Introduction

Precision oncology has transformed cancer treatment by replacing uniform therapeutic strategies with individualized interventions guided by molecular biology, tumor characteristics, and patient-specific clinical information. Nevertheless, predicting therapeutic response remains a major challenge because

cancer is characterized by continuous genomic evolution, epigenetic remodeling, immune adaptation, metabolic reprogramming, and interactions within the tumor microenvironment.[2]

Modern oncology generates enormous quantities of heterogeneous biomedical information through radiological imaging, digital pathology, genomic

sequencing, transcriptomics, proteomics, metabolomics, spatial transcriptomics, laboratory investigations, wearable technologies, liquid biopsy, and electronic health records. Although each modality provides valuable biological insight, isolated analysis often fails to capture the complex interactions underlying therapeutic response and resistance.[3]

Foundation artificial intelligence models have emerged as transformative computational frameworks capable of integrating these diverse biomedical modalities into generalized patient-specific representations. By combining self-supervised learning, multimodal transformers, graph neural networks, and generative AI, foundation models provide unprecedented opportunities for predictive therapeutics, biomarker discovery, adaptive treatment planning, and precision clinical decision-making.[4]

The convergence of foundation AI models with translational oncology is therefore redefining predictive cancer therapeutics by enabling increasingly accurate, personalized, and continuously adaptive treatment strategies.[5]

2.Evolution of Predictive Cancer Therapeutics

Historically, therapeutic decisions in oncology were based primarily on tumor histology, anatomical staging, and standardized treatment protocols. Although these approaches significantly improved cancer management, substantial variability in therapeutic response remained because biological heterogeneity was incompletely understood.[6]

Advances in molecular oncology introduced genomic biomarkers, targeted therapies, immune checkpoint inhibitors, and precision medicine, enabling increasingly individualized treatment selection. High-throughput sequencing technologies further expanded biological understanding through transcriptomics, proteomics, metabolomics, epigenomics, and single-cell analyses.

Artificial intelligence subsequently enabled computational interpretation of these complex datasets, while foundation AI models introduced generalized biomedical representation learning capable of transferring knowledge across multiple malignancies and therapeutic applications.

Today, predictive therapeutics extends beyond isolated biomarkers toward integrated computational ecosystems capable of modeling complex biological interactions throughout the cancer continuum.[7]

3.Foundation AI Models in Precision Therapeutics

Foundation AI models differ fundamentally from conventional machine learning algorithms because they are pretrained on massive multimodal biomedical datasets before adaptation to specialized oncology tasks. Rather than learning individual prediction problems, these models acquire generalized biological representations applicable across diagnosis, prognosis, biomarker discovery, therapeutic response prediction, and clinical decision support.[8]

Self-supervised learning enables discovery of latent biological relationships without extensive manual annotation, while transformer architectures efficiently integrate radiological imaging, digital pathology, genomic sequencing, transcriptomics, proteomics, metabolomics, laboratory biomarkers, and electronic health records into unified computational embeddings.

Graph neural networks further strengthen biological reasoning by modeling interactions among genes, proteins, signaling pathways, immune populations, metabolites, therapeutic targets, and clinical outcomes. These computational approaches substantially improve transfer learning, robustness, and generalizability across diverse oncology applications.[9]

4.Computational Architecture

Modern predictive therapeutic platforms consist of interconnected computational layers responsible for multimodal biomedical data acquisition, preprocessing, representation learning, predictive analytics, adaptive model refinement, and intelligent clinical decision support.[10]

The acquisition layer continuously integrates radiological imaging, digital pathology, genomic sequencing, transcriptomics, proteomics, metabolomics, spatial biology, laboratory biomarkers, wearable sensor information, medication history, liquid biopsy, and longitudinal electronic health records. Advanced preprocessing

pipelines normalize imaging studies, harmonize molecular datasets, encode clinical narratives using natural language processing, and synchronize temporal patient information.

Transformer-based foundation models generate generalized computational embeddings representing molecular biology, tissue architecture, imaging phenotypes, physiological status, and clinical trajectories. Graph neural networks model relationships among molecular pathways, cellular communication networks, immune responses, therapeutic targets, and treatment outcomes, enabling systems-level predictive reasoning.[11]

5. Artificial Intelligence for Biomarker Discovery

Biomarker discovery remains one of the most important applications of foundation AI models because predictive biomarkers are essential for selecting optimal therapies and identifying patients most likely to benefit from precision medicine. Conventional biomarker discovery frequently relies on isolated genomic analyses, whereas foundation AI models integrate heterogeneous biomedical information across multiple biological scales.[12]

Artificial intelligence identifies complex nonlinear relationships among genomic alterations, transcriptomic signatures, proteomic profiles, metabolomic pathways, spatial biology, imaging phenotypes, histopathological architecture, and longitudinal clinical outcomes. Machine learning automatically detects latent biological features associated with therapeutic sensitivity, resistance, toxicity, recurrence, and survival.

These computational approaches accelerate identification of novel diagnostic, prognostic, predictive, pharmacodynamic, and companion biomarkers while substantially improving individualized therapeutic stratification.[13]

6. Multi-Omics Integration and Therapeutic Prediction

Foundation AI models increasingly depend upon comprehensive integration of genomics, transcriptomics, proteomics, metabolomics, epigenomics, lipidomics, immunomics, microbiomics, and single-cell sequencing into unified molecular representations of tumor biology.[14]

Multimodal transformers, biological knowledge graphs, and graph neural networks identify interactions among genes, proteins, metabolites, immune pathways, signaling cascades, and therapeutic targets that cannot be detected through isolated molecular analyses.

These integrated computational representations improve molecular subtype classification, drug sensitivity prediction, biomarker discovery, immunotherapy selection, and personalized treatment planning while strengthening systems-level understanding of cancer biology.[15]

7. Digital Pathology and Imaging Biomarkers

Digital pathology and radiological imaging provide complementary phenotypic information describing tumor biology across multiple spatial scales. Foundation AI models trained on whole-slide images automatically learn generalized histomorphological representations, whereas multimodal imaging models characterize tumor morphology, vascularity, metabolism, perfusion, and metastatic dissemination.[16]

Artificial intelligence integrates radiomics, computational pathology, molecular biology, laboratory biomarkers, and clinical outcomes into unified computational frameworks capable of predicting therapeutic biomarkers directly from routine imaging studies and histopathological slides.

These multimodal imaging biomarkers substantially improve diagnosis, prognostic prediction, molecular characterization, immunotherapy selection, and precision therapeutic planning while reducing dependence on invasive diagnostic procedures.[17]

8. Predictive Modeling of Therapeutic Response

One of the most clinically significant applications of foundation AI models is accurate prediction of therapeutic response across chemotherapy, targeted therapy, endocrine therapy, immunotherapy, radiation therapy, surgery, and multimodal treatment combinations. Unlike conventional statistical models, foundation AI systems simultaneously analyze imaging, pathology, molecular biology, laboratory investigations, medication history, physiological monitoring, and longitudinal clinical trajectories.[18]

These intelligent computational models estimate treatment efficacy, progression-free survival, overall survival, recurrence probability, treatment-related toxicity, and mechanisms of therapeutic resistance while continuously adapting predictions using newly acquired clinical evidence. Such predictive capabilities support personalized therapeutic optimization throughout the patient's cancer journey.[19]

9.Clinical Translation and Precision Medicine

The ultimate objective of predictive cancer therapeutics is successful translation of computational discoveries into routine clinical practice. Foundation AI models facilitate this transition by integrating multimodal biomedical information into intelligent clinical decision-support systems capable of providing individualized therapeutic recommendations while supporting multidisciplinary oncology teams.[20]

10.Digital Twins and Virtual Therapeutic Simulation

Digital twin technology represents one of the most promising applications of foundation AI models in predictive cancer therapeutics. AI-powered digital twins integrate radiological imaging, digital pathology, genomics, transcriptomics, proteomics, metabolomics, laboratory biomarkers, liquid biopsy, wearable physiological monitoring, treatment history, and longitudinal clinical outcomes into continuously evolving virtual patient models.[21]

These computational replicas remain synchronized with biological patients throughout diagnosis, treatment, follow-up, and survivorship. Foundation AI models simulate tumor evolution, immune responses, therapeutic efficacy, drug resistance, treatment-related toxicity, recurrence, and metastatic progression under multiple therapeutic scenarios before actual clinical intervention. Such virtual simulations enable clinicians to compare alternative treatment strategies, optimize therapeutic sequencing, and personalize interventions while minimizing unnecessary toxicity and maximizing clinical benefit.

11.Foundation Models for Drug Discovery and Target Identification

The application of foundation AI models extends beyond clinical prediction into drug discovery and therapeutic target identification. Modern transformer architectures integrate multi-omics datasets, structural biology, protein interaction networks, chemical libraries, and pharmacological databases to identify novel therapeutic targets associated with tumor progression and resistance mechanisms.[22]

Artificial intelligence predicts protein structures, ligand-binding interactions, signaling pathway perturbations, synthetic lethality relationships, and pharmacodynamic responses while accelerating the discovery of candidate therapeutic compounds. Generative AI further supports rational drug design by creating chemically plausible molecular structures optimized for specific biological targets.

These computational approaches substantially reduce the time, cost, and complexity of preclinical drug development while improving the likelihood of successful clinical translation.

12.Adaptive Therapeutic Optimization

Cancer therapy requires continuous adaptation because tumor biology evolves through clonal selection, genomic instability, immune escape, metabolic reprogramming, and treatment-induced resistance. Foundation AI models address this challenge by continuously integrating longitudinal patient information into adaptive computational frameworks capable of updating therapeutic recommendations throughout disease progression.[23]

Artificial intelligence analyzes imaging studies, computational pathology, circulating tumor DNA, laboratory biomarkers, wearable physiological monitoring, medication adherence, and real-world clinical outcomes to estimate treatment efficacy and identify emerging resistance before overt clinical progression becomes apparent.

This adaptive therapeutic optimization enables personalized treatment modifications, dose adjustments, combination therapy selection, and dynamic sequencing of therapeutic interventions according to evolving patient-specific biology.

13. Intelligent Clinical Decision Support

Foundation AI models provide the computational core for next-generation clinical decision-support systems in predictive oncology. These intelligent platforms integrate radiological imaging, digital pathology, molecular diagnostics, laboratory investigations, electronic health records, medication history, wearable technologies, and evidence-based clinical guidelines into comprehensive patient-centered computational environments.[24]

Interactive clinical dashboards generate individualized diagnostic summaries, molecular interpretations, biomarker analyses, therapeutic recommendations, toxicity estimates, recurrence predictions, and survival probabilities while facilitating multidisciplinary collaboration among oncologists, radiologists, pathologists, surgeons, molecular biologists, pharmacists, and bioinformaticians.

Such intelligent decision-support systems enhance workflow efficiency, reduce fragmentation of biomedical information, improve diagnostic consistency, and promote evidence-based precision medicine throughout the oncology care continuum.

14. Explainability, Validation, and Regulatory Considerations

Despite remarkable advances in predictive therapeutics, successful implementation of foundation AI models requires transparency, interpretability, reproducibility, and rigorous scientific validation. Explainable artificial intelligence (XAI) enables clinicians to understand computational reasoning through attention visualization, saliency maps, SHAP (Shapley Additive Explanations), feature attribution analysis, uncertainty estimation, and counterfactual explanations that identify the biological variables contributing most strongly to AI-generated therapeutic recommendations.[25]

Clinical implementation also requires standardized multimodal datasets, interoperable computational infrastructure, prospective multicenter validation, external benchmarking, continuous monitoring for algorithmic bias, cybersecurity safeguards, and compliance with evolving international regulatory

frameworks governing AI-enabled medical technologies.

Responsible governance emphasizing patient privacy, informed consent, equitable access, transparency, accountability, and continuous post-deployment monitoring will remain fundamental for trustworthy clinical translation.

15. Future Perspectives

Future predictive cancer therapeutics will increasingly integrate multimodal foundation models, agentic artificial intelligence, large language models, federated learning, reinforcement learning, retrieval-augmented generation, digital twins, spatial multi-omics, liquid biopsy, quantum computing, cloud-native healthcare infrastructure, and Internet of Medical Things (IoMT) technologies into unified intelligent oncology ecosystems.[26]

These next-generation computational platforms will continuously assimilate molecular biology, imaging, pathology, laboratory medicine, physiological monitoring, environmental exposures, electronic health records, and real-world clinical outcomes while autonomously coordinating diagnostic workflows, optimizing therapeutic strategies, generating personalized patient education, and supporting continuous biomedical evidence synthesis.

Such integrated AI ecosystems are expected to transform predictive therapeutics from static treatment planning toward continuously adaptive, learning healthcare systems capable of delivering truly individualized cancer care.

16. Discussion

Foundation AI models represent a transformative advancement in predictive cancer therapeutics by integrating molecular biology, cellular phenotypes, tissue architecture, radiological imaging, laboratory biomarkers, and longitudinal clinical intelligence into unified computational representations. Unlike conventional task-specific algorithms, these models provide generalized biomedical reasoning capable of supporting biomarker discovery, therapeutic response prediction, adaptive treatment optimization, digital twins, intelligent clinical decision support, and translational oncology research.[27]

Applications spanning computational pathology, radiogenomics, multi-omics integration, systems oncology, precision immunotherapy, virtual therapeutic simulation, and AI-assisted drug discovery demonstrate the extraordinary potential of foundation models to accelerate clinical translation. Nevertheless, widespread implementation requires continued advances in multimodal data harmonization, explainable artificial intelligence, interoperability, computational infrastructure, regulatory science, cybersecurity, ethical governance, and multidisciplinary collaboration.

As increasingly comprehensive biomedical datasets become available, foundation AI models will serve as the computational backbone of predictive precision oncology.

17. Conclusion

Foundation AI models are redefining predictive cancer therapeutics by integrating multimodal biomedical information into intelligent computational frameworks capable of supporting biomarker discovery, molecular characterization, therapeutic response prediction, adaptive treatment optimization, drug discovery, digital twins, and personalized clinical decision-making across the entire cancer care continuum.[28]

Advances in transformer architectures, multimodal learning, graph neural networks, self-supervised learning, federated learning, reinforcement learning, large language models, agentic AI, and generative artificial intelligence are expected to further strengthen predictive computational oncology, enabling increasingly accurate diagnosis, individualized therapeutic planning, continuous disease monitoring, and evidence-based clinical translation.[29]

Although important scientific, technical, ethical, regulatory, and implementation challenges remain, sustained collaboration among oncologists, pathologists, radiologists, molecular biologists, biomedical engineers, computer scientists, healthcare organizations, pharmaceutical industries, and regulatory agencies will accelerate the responsible adoption of foundation AI models. These innovations have the potential to improve patient outcomes, enhance therapeutic precision, reduce healthcare disparities, and establish a new

era of intelligent, predictive, and personalized cancer medicine worldwide.[30]

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