



ARTIFICIAL INTELLIGENCE–DRIVEN CANCER KNOWLEDGE GRAPHS FOR PRECISION DIAGNOSIS AND THERAPEUTIC DISCOVERY

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Abstract: Artificial intelligence (AI)-driven cancer knowledge graphs are emerging as a transformative computational paradigm for precision oncology by integrating heterogeneous biomedical information into structured, interconnected representations of cancer biology. Conventional oncology workflows frequently analyze radiological imaging, digital pathology, genomics, transcriptomics, proteomics, metabolomics, epigenomics, laboratory investigations, biomedical literature, electronic health records, and clinical guidelines independently, limiting comprehensive understanding of molecular mechanisms and therapeutic opportunities. Recent advances in foundation AI models, graph neural networks, multimodal transformer architectures, self-supervised learning, reinforcement learning, retrieval-augmented generation, and generative artificial intelligence have enabled construction of dynamic cancer knowledge graphs capable of integrating genes, proteins, signaling pathways, biomarkers, imaging phenotypes, histopathological characteristics, therapeutic agents, clinical trials, digital biomarkers, patient outcomes, and biomedical evidence into unified computational ecosystems. These intelligent systems support precision diagnosis, biomarker discovery, molecular pathway analysis, drug target identification, therapeutic optimization, drug repurposing, adaptive clinical trials, digital twin simulation, and evidence-based clinical decision support. Emerging technologies including multimodal large language models, federated learning, explainable artificial intelligence, agentic AI, cloud-native healthcare platforms, and digital health ecosystems further strengthen cancer knowledge graphs by enabling collaborative, privacy-preserving, transparent, and continuously adaptive biomedical intelligence. Despite remarkable technological progress, important scientific, technical, ethical, and regulatory challenges remain regarding knowledge harmonization, computational scalability, interoperability, data quality, cybersecurity, clinical validation, regulatory acceptance, and equitable implementation. This review provides a comprehensive overview of AI-driven cancer knowledge graphs, emphasizing their role in precision diagnosis and therapeutic discovery for next-generation oncology.[1]

Keywords: *Cancer knowledge graphs, Foundation models, Graph neural networks, Artificial intelligence, Precision oncology, Therapeutic discovery, Computational oncology, Clinical decision support, Precision medicine, Biomedical knowledge.*

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1. Introduction

Cancer is a biologically complex disease characterized by dynamic interactions among genomic alterations, epigenetic regulation, transcriptomic activity, proteomic signaling, metabolic remodeling, immune adaptation, stromal interactions, vascular biology, and environmental influences. These interconnected biological

mechanisms evolve continuously throughout diagnosis, treatment, recurrence, metastasis, and survivorship, making precision oncology increasingly dependent upon computational systems capable of integrating heterogeneous biomedical information into coherent biological representations.[2]

Modern oncology generates enormous quantities of biomedical information through radiological imaging, digital pathology, genomic sequencing, transcriptomics, proteomics, metabolomics, epigenomics, spatial biology, laboratory investigations, circulating tumor DNA, wearable physiological monitoring, physician documentation, electronic health records, biomedical literature, drug databases, clinical guidelines, and patient-reported outcomes. Although each modality contributes valuable biological insight, isolated interpretation frequently limits comprehensive understanding of disease mechanisms and individualized therapeutic decision-making.[3]

Artificial intelligence-driven cancer knowledge graphs address these limitations by organizing diverse biomedical entities and their relationships into structured computational networks capable of supporting precision diagnosis, biomarker discovery, therapeutic optimization, translational research, and personalized cancer medicine.

2. Evolution of Cancer Knowledge Graphs

Biomedical knowledge representation has evolved from manually curated databases toward intelligent graph-based computational ecosystems capable of integrating multimodal biomedical information. Early biomedical databases primarily stored isolated molecular annotations, pathway information, drug interactions, and clinical evidence using relational database architectures. Although these resources significantly advanced biomedical research, they frequently lacked dynamic integration across heterogeneous biomedical domains.[4]

Graph databases subsequently enabled representation of complex biological relationships among genes, proteins, metabolites, signaling pathways, diseases, drugs, and clinical outcomes. Deep learning and graph neural networks further expanded computational capabilities by enabling automated inference across large-scale biological networks.

Foundation AI models now acquire transferable biomedical knowledge through multimodal self-supervised learning, enabling dynamic construction, refinement, and reasoning across continuously

evolving cancer knowledge graphs supporting precision oncology.[5]

3. Principles of AI-Driven Cancer Knowledge Graphs

Cancer knowledge graphs differ fundamentally from conventional biomedical databases because they represent biological entities and their relationships within interconnected graph structures that support intelligent reasoning and knowledge discovery. Rather than storing isolated biomedical variables, graph-based systems integrate genes, proteins, signaling pathways, molecular biomarkers, radiological imaging phenotypes, histopathological features, therapeutic agents, clinical trials, environmental exposures, physiological variables, and patient outcomes into unified computational networks.[6]

Foundation AI models acquire generalized graph representations through self-supervised learning, while graph neural networks propagate biological information across interconnected nodes to identify latent relationships that may not be directly observable. Multimodal transformer architectures simultaneously align radiological imaging, digital pathology, genomics, transcriptomics, proteomics, metabolomics, laboratory biomarkers, biomedical literature, physician documentation, and longitudinal clinical trajectories within shared computational embedding spaces.

These computational principles establish dynamic knowledge ecosystems capable of supporting systems-level reasoning throughout precision oncology.[7]

4. Computational Architecture

Modern AI-driven cancer knowledge graph platforms consist of interconnected computational layers responsible for biomedical data acquisition, knowledge extraction, entity recognition, relationship discovery, graph construction, multimodal representation learning, graph reasoning, predictive analytics, digital twin simulation, and intelligent clinical decision support.[8]

The acquisition layer continuously integrates radiological imaging, digital pathology, genomic sequencing, transcriptomics, proteomics, metabolomics, epigenomics, laboratory investigations, circulating tumor DNA, wearable physiological monitoring, medication history, physician documentation, biomedical literature, clinical guidelines, pharmacological databases, and electronic health records. Natural language processing extracts biomedical entities from scientific publications and clinical documentation, while graph construction algorithms establish semantic relationships among diverse biomedical concepts.

Foundation AI models subsequently generate generalized graph embeddings representing molecular biology, imaging phenotypes, tissue architecture, physiological function, pharmacological mechanisms, environmental exposures, and longitudinal clinical trajectories, thereby enabling adaptive knowledge reasoning throughout precision oncology.[9]

5. Knowledge Graphs for Precision Diagnosis

One of the most important applications of AI-driven cancer knowledge graphs is precision diagnosis through comprehensive integration of multimodal biomedical evidence. Foundation AI models combine radiological imaging, digital pathology, molecular biomarkers, laboratory investigations, genomic alterations, physician documentation, biomedical literature, and clinical guidelines into structured graph representations supporting comprehensive diagnostic reasoning.[10]

Graph neural networks identify biologically meaningful relationships among imaging features, histopathological architecture, molecular alterations, immune phenotypes, laboratory biomarkers, and disease subtypes while simultaneously incorporating evidence from scientific publications and real-world clinical outcomes. Retrieval-augmented generation further enables contextual interpretation of complex biomedical evidence using continuously updated scientific knowledge.

These computational approaches substantially improve diagnostic accuracy, molecular classification, biomarker interpretation, and personalized oncology.[11]

6. Therapeutic Discovery Through Graph Intelligence

Cancer knowledge graphs have become powerful computational tools for therapeutic discovery by integrating molecular biology, pharmacology, signaling pathways, protein interactions, drug mechanisms, clinical trials, treatment outcomes, and biomedical literature into interconnected biological networks. Foundation AI models identify novel therapeutic targets, drug-gene interactions, pathway vulnerabilities, synthetic lethal relationships, resistance mechanisms, and opportunities for drug repurposing through graph-based reasoning.[12]

Graph neural networks propagate biological information across interconnected molecular networks while transformer architectures integrate multimodal biomedical evidence into generalized therapeutic representations. These systems continuously synthesize emerging scientific evidence, enabling adaptive identification of promising therapeutic hypotheses for experimental validation.

Such graph-based computational intelligence substantially accelerates translational oncology research, precision drug discovery, and personalized therapeutic development.[13]

7. Multi-Omics Knowledge Integration

Comprehensive characterization of cancer biology requires integration of complementary molecular technologies including genomics, transcriptomics, proteomics, metabolomics, epigenomics, immunomics, microbiomics, single-cell sequencing, spatial transcriptomics, and spatial proteomics. AI-driven knowledge graphs harmonize these diverse molecular modalities using graph neural networks and multimodal transformer architectures capable of generating generalized biological representations of evolving tumor ecosystems.[14]

Artificial intelligence identifies latent biological relationships among genes, proteins, metabolites,

signaling pathways, immune responses, epigenetic regulation, imaging phenotypes, histopathological architecture, and therapeutic targets while continuously updating graph structures according to emerging biomedical evidence.

These integrated graph representations substantially improve biomarker discovery, molecular classification, therapeutic selection, precision immunotherapy, adaptive therapeutics, and translational cancer research.[15]

8. Biomedical Literature and Clinical Knowledge Integration

The biomedical literature continues to expand at an unprecedented pace, making comprehensive evidence synthesis increasingly difficult for clinicians and researchers. AI-driven cancer knowledge graphs automatically extract biomedical entities, molecular relationships, therapeutic evidence, adverse events, clinical trial findings, pharmacological mechanisms, and guideline recommendations from scientific publications using natural language processing and large language models.[16]

Retrieved evidence is integrated with radiological imaging, digital pathology, molecular diagnostics, electronic health records, laboratory investigations, and real-world clinical outcomes to generate continuously evolving biomedical knowledge networks. Retrieval-augmented generation further enables context-aware interpretation of scientific literature while reducing hallucination and improving evidence traceability.

These capabilities substantially strengthen precision diagnosis, therapeutic discovery, clinical decision support, and translational oncology research.[17]

9. Knowledge Graph–Driven Clinical Intelligence

One of the greatest strengths of AI-driven cancer knowledge graphs is their ability to unify radiology, pathology, multi-omics, pharmacological knowledge, biomedical literature, clinical guidelines, electronic health records, laboratory biomarkers, digital biomarkers, patient-reported outcomes, and longitudinal clinical trajectories into

comprehensive patient-specific computational representations. Rather than analyzing individual biomedical modalities independently, these graph-based systems generate holistic representations of evolving cancer biology capable of supporting diagnosis, biomarker discovery, therapeutic optimization, disease monitoring, recurrence prediction, survival estimation, multidisciplinary communication, and precision clinical decision-making. This graph-centered intelligence establishes the computational foundation for adaptive precision oncology, digital twins, intelligent clinical decision support, and continuously personalized cancer care throughout the cancer care continuum.[18][19][20]

10. Digital Twins and Knowledge Graph–Driven Patient Modeling

Digital twin technology represents one of the most transformative applications of AI-driven cancer knowledge graphs by creating continuously evolving virtual representations of individual cancer patients synchronized with their biological counterparts. Foundation AI models integrate serial radiological imaging, digital pathology, genomics, transcriptomics, proteomics, metabolomics, epigenomics, spatial biology, laboratory biomarkers, circulating tumor DNA, wearable physiological monitoring, medication history, patient-reported outcomes, and longitudinal clinical information into adaptive computational patient models capable of simulating disease progression, therapeutic response, treatment-related toxicity, recurrence, metastatic dissemination, and survival.[21]

Unlike conventional predictive models, digital twins continuously update their computational representations as new biomedical information becomes available. Cancer knowledge graphs organize molecular pathways, pharmacological interactions, signaling networks, clinical guidelines, imaging phenotypes, pathological findings, and therapeutic evidence into structured semantic relationships that continuously inform digital twin simulations. These graph-enhanced virtual patients enable evaluation of multiple therapeutic strategies,

optimization of treatment sequencing, prediction of resistance mechanisms, personalization of supportive care, and estimation of long-term clinical outcomes according to evolving patient biology.

By integrating graph reasoning with predictive simulation, digital twins transform computational oncology from retrospective analysis toward proactive, adaptive, and continuously personalized precision medicine.

11. Intelligent Clinical Decision Support

Cancer knowledge graphs provide the computational infrastructure for next-generation clinical decision-support systems capable of integrating heterogeneous biomedical information into comprehensive patient-centered recommendations. Rather than independently interpreting radiological imaging, digital pathology, molecular diagnostics, laboratory investigations, wearable physiological monitoring, medication history, physician documentation, patient-reported outcomes, and evidence-based clinical guidelines, graph-based intelligence synthesizes diverse biomedical information into unified computational representations supporting multidisciplinary oncology practice.[22]

Interactive clinical dashboards generate individualized diagnostic summaries, molecular biomarker analyses, graph-derived pathway interpretations, digital twin simulations, therapeutic recommendations, toxicity estimates, recurrence probabilities, disease progression forecasts, survival predictions, drug interaction analyses, and longitudinal treatment response assessments while facilitating collaboration among oncologists, radiologists, pathologists, surgeons, radiation oncologists, molecular biologists, pharmacists, nurses, genetic counselors, biomedical engineers, computational scientists, and healthcare administrators.

These intelligent systems improve workflow efficiency, strengthen multidisciplinary communication, reduce fragmentation of biomedical information, and promote evidence-based personalized cancer management throughout the cancer care continuum.

12. Continuous Learning and Adaptive Knowledge Graphs

A defining characteristic of AI-driven cancer knowledge graphs is the ability to continuously evolve as new biomedical information becomes available. Artificial intelligence incorporates newly published biomedical literature, serial imaging examinations, computational pathology, circulating tumor DNA, laboratory biomarkers, wearable physiological monitoring, medication adherence, patient-reported outcomes, pharmacological evidence, clinical guidelines, and real-world clinical outcomes into adaptive graph structures capable of continuously refining predictive accuracy throughout the patient's clinical journey.[23]

Continual learning algorithms enable incremental refinement of graph representations without catastrophic forgetting of previously acquired knowledge, while reinforcement learning optimizes diagnostic reasoning, therapeutic recommendations, pathway interpretation, and biomarker prioritization through iterative evaluation of longitudinal patient outcomes. Foundation AI models further integrate clinician feedback and multidisciplinary tumor board recommendations into continuous graph refinement.

This adaptive computational paradigm transforms oncology into a continuously learning knowledge ecosystem capable of rapidly translating scientific discoveries into individualized clinical practice.

13. Federated Cancer Knowledge Graph Networks

Development of highly generalizable cancer knowledge graphs requires access to diverse biomedical datasets representing multiple healthcare systems, imaging platforms, pathology laboratories, molecular technologies, pharmacological databases, wearable ecosystems, treatment protocols, and patient populations. Federated learning enables collaborative development of graph-based clinical intelligence while preserving patient privacy and institutional governance through decentralized computational training.[24]

Participating healthcare institutions independently construct local cancer knowledge graphs using

radiological imaging, digital pathology, genomics, transcriptomics, proteomics, laboratory investigations, wearable monitoring, liquid biopsy, electronic health records, biomedical literature, and longitudinal clinical records while securely exchanging encrypted graph representations and model parameters rather than identifiable patient information. This collaborative learning strategy substantially improves algorithm robustness, fairness, external validity, transparency, and generalizability across diverse healthcare environments.

Federated cancer knowledge graph ecosystems therefore establish international computational oncology networks capable of accelerating scientific discovery, improving equitable access to precision medicine, reducing institutional bias, and supporting global cancer research while maintaining responsible biomedical data stewardship.

14. Explainability, Validation, and Ethical Governance

Successful implementation of AI-driven cancer knowledge graphs requires transparent, interpretable, reproducible, and rigorously validated computational systems capable of supporting clinician confidence, patient trust, and regulatory approval. Explainable artificial intelligence (XAI) enables clinicians to understand graph-based computational reasoning through pathway visualization, graph attention mechanisms, saliency maps, SHAP (Shapley Additive Explanations), feature attribution analysis, uncertainty estimation, confidence calibration, and counterfactual explanations identifying the molecular, pathological, imaging, physiological, pharmacological, and clinical variables responsible for predictive outputs.[25]

Clinical deployment additionally requires standardized biomedical ontologies, interoperable graph databases, prospective multicenter validation, external benchmarking, cybersecurity safeguards, continuous monitoring for algorithmic bias, transparent reporting standards, and compliance with evolving international regulatory frameworks governing AI-enabled healthcare technologies.

Responsible implementation further depends upon patient privacy, informed consent, transparency, accountability, fairness, equitable access, responsible data governance, continuous post-deployment surveillance, clinician education, and multidisciplinary oversight to ensure trustworthy integration of cancer knowledge graphs into routine oncology practice.

15. Future Perspectives

Future cancer knowledge graph ecosystems will increasingly integrate multimodal foundation models, multimodal large language models, agentic artificial intelligence, graph neural networks, reinforcement learning, federated learning, digital twins, spatial multi-omics, single-cell sequencing, liquid biopsy, quantum computing, Internet of Medical Things (IoMT), robotics, cloud-native healthcare infrastructure, biomedical knowledge graphs, autonomous reasoning systems, and retrieval-augmented generation into unified precision oncology platforms.[26]

These next-generation computational ecosystems will continuously integrate molecular biology, radiological imaging, digital pathology, laboratory medicine, wearable physiological monitoring, environmental exposures, electronic health records, biomedical literature, pharmacological databases, global clinical guidelines, and real-world clinical outcomes while autonomously coordinating knowledge synthesis, biomarker discovery, therapeutic prioritization, adaptive clinical trials, personalized therapeutics, survivorship management, and continuous evidence generation. Such intelligent knowledge ecosystems are expected to transform oncology from fragmented information management toward predictive, adaptive, continuously learning, graph-centered precision medicine across the global cancer community.

16. Discussion

AI-driven cancer knowledge graphs represent one of the most significant paradigm shifts in computational oncology by integrating molecular biology, radiology, pathology, pharmacology,

biomedical literature, clinical guidelines, laboratory biomarkers, digital biomarkers, digital twins, and foundation AI models into unified computational ecosystems capable of supporting comprehensive personalized cancer care. Unlike conventional biomedical databases that store isolated information, graph-based intelligence continuously synthesizes heterogeneous molecular, imaging, pathological, physiological, pharmacological, and clinical information into interconnected biological networks that support systems-level reasoning and therapeutic discovery.[27]

Applications spanning computational pathology, radiogenomics, biomarker discovery, drug repurposing, digital twins, precision immunotherapy, adaptive therapeutics, remote patient monitoring, continuous learning, federated collaboration, digital health, survivorship management, and intelligent clinical decision support demonstrate the extraordinary potential of cancer knowledge graphs to redefine future oncology. Nevertheless, successful implementation requires continued advances in knowledge harmonization, explainable artificial intelligence, interoperability, computational infrastructure, cybersecurity, regulatory science, ethical governance, clinician education, and sustained multidisciplinary collaboration.

As biomedical knowledge and healthcare data continue to expand exponentially, AI-driven cancer knowledge graphs are expected to become one of the foundational computational infrastructures supporting precision oncology worldwide.

17. Conclusion

Artificial intelligence-driven cancer knowledge graphs are transforming precision oncology by integrating radiological imaging, digital pathology, multi-omics, pharmacological knowledge, biomedical literature, laboratory biomarkers, electronic health records, digital biomarkers, digital twins, and longitudinal clinical intelligence into unified computational ecosystems capable of supporting accurate diagnosis, biomarker discovery, molecular pathway analysis, therapeutic optimization, adaptive disease monitoring, and

personalized therapeutics throughout the cancer care continuum.[28]

Advances in foundation AI models, graph neural networks, multimodal learning, self-supervised learning, federated learning, reinforcement learning, digital twins, multimodal large language models, agentic AI, retrieval-augmented generation, and generative artificial intelligence are expected to further strengthen graph-centered oncology ecosystems, enabling increasingly accurate molecular characterization, predictive clinical reasoning, adaptive therapeutics, continuous knowledge synthesis, and precision drug discovery.[29]

Although important scientific, technical, ethical, regulatory, and implementation challenges remain, sustained collaboration among oncologists, radiologists, pathologists, molecular biologists, biomedical engineers, pharmacologists, computer scientists, healthcare organizations, policymakers, industry partners, patients, and regulatory agencies will accelerate the responsible implementation of AI-driven cancer knowledge graphs. These innovations have the potential to improve patient outcomes, enhance healthcare efficiency, reduce disparities in cancer care, accelerate translational research, facilitate therapeutic discovery, and establish a new era of intelligent, adaptive, and continuously learning precision oncology worldwide.[30]

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