



Review Article

Artificial Intelligence for Drug Repurposing and Target Discovery in Oncology

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Cancer remains a leading cause of morbidity and mortality globally, with conventional drug discovery facing significant challenges including high development costs, prolonged timelines, and substantial failure rates. Artificial intelligence (AI), encompassing machine learning (ML) and deep learning (DL) approaches, has emerged as a transformative technology for accelerating oncology drug discovery and enabling precision medicine. This review synthesizes recent advances (2020–2026) in AI-driven drug repurposing and target identification in cancer research. We examine how AI integrates multi-omics data—including genomics, transcriptomics, proteomics, and radiomics—to predict drug–target interactions, identify novel therapeutic targets, and uncover repurposing opportunities for existing drugs. Key methods discussed include supervised and unsupervised machine learning, graph neural networks (GNNs), deep neural networks (DNNs), and transformer-based architectures. Applications across multiple cancer types demonstrate that AI-enabled approaches significantly reduce discovery timelines and costs while improving prediction accuracy. However, substantial challenges persist, including data heterogeneity, model interpretability, clinical translation barriers, and regulatory uncertainties. This review highlights that despite these limitations, AI-driven oncology drug discovery represents a paradigm shift toward faster, more cost-effective identification of therapeutic candidates and biomarkers. Future directions emphasize explainable AI (XAI), federated learning for privacy preservation, and rigorous prospective clinical validation to realize AI's full potential in precision cancer medicine.

Keywords: artificial intelligence, machine learning, deep learning, drug repurposing, target discovery, oncology, drug–target interaction, precision medicine, biomarker discovery, graph neural networks.

INTRODUCTION

Cancer diagnosis and treatment face significant global challenges, with artificial intelligence (AI) transforming drug discovery by enabling the rapid identification of existing drugs with potential anti-cancer properties through drug repurposing, offering a cost-effective and time-efficient alternative to traditional drug development. (1) Despite conventional drug discovery methods proving time-consuming, costly, and often ineffective in tackling the complexity and heterogeneity of malignancies, AI has significantly improved the prediction of molecular properties, reduced attrition rates, and enabled the repurposing of existing drugs for new

cancer indications. (2) The development of effective anticancer therapies remains one of the most pressing challenges in modern medicine. Cancer accounts for an estimated 9.6 million deaths annually, and certain cancers such as pancreatic and gastric cancers are detected only after reaching advanced stages with frequent relapses. (3) Traditional drug discovery pipelines typically require 10–15 years and investments exceeding US\$2.6 billion per approved drug, with less than 10% of compounds entering clinical trials ultimately achieving regulatory approval. Drug discovery is adapting to novel technologies such as data science, informatics, and

artificial intelligence to accelerate effective treatment development while reducing costs and animal experiments. (4) Drug repurposing provides a cost-effective strategy to re-use approved drugs for new medical indications, with several machine learning and artificial intelligence approaches developed for systematic identification of drug repurposing leads based on big data resources, further accelerating and de-risking the drug development process by computational means. (5) Repurposing non-oncology small-molecule drugs has been increasingly becoming an attractive approach to improve cancer therapy, with potentially lower overall costs and shorter timelines, facilitated by emerging technologies such as omics sequencing and artificial intelligence. (6) AI enables precise target identification, accelerates virtual drug screening and molecular design, and enhances clinical trial efficiency through intelligent patient stratification and adaptive protocols, while facilitating personalized treatment decision-making, early prediction of drug resistance, and real-time toxicity surveillance. (7) By integrating comprehensive multi-omics datasets spanning genomic, transcriptomic, proteomic, and epigenomic profiles with clinical response data, sophisticated machine learning models can identify novel biomarker signatures correlating with differential drug sensitivity across a spectrum of cancer types. (8) The integration of AI with multi-dimensional biological data represents a paradigm shift in oncology research. Artificial intelligence based on big data can extract hidden patterns, important information, and corresponding knowledge behind enormous amounts of data, enabling machine learning and deep learning to mine deep-level information in genomics, transcriptomics, proteomics, radiomics, and digital pathological images to provide comprehensive understanding of tumors and personalized treatments. (9) Artificial intelligence provides a quantitative framework to study the relationship between network characteristics and cancer through network-based and machine learning-based approaches, thereby leading to the identification of potential anticancer targets and the discovery of novel drug candidates. (10) This comprehensive review synthesizes recent literature (2020–2026) on AI applications in oncology drug repurposing and target discovery, evaluating methodologies, successful applications, current

limitations, and future perspectives for translating computational predictions into clinical benefit.

2. Overview of Artificial Intelligence in Oncology Drug Discovery

AI encompasses a diverse set of computational methodologies designed to enable machines to learn patterns from data and make predictions or decisions. Machine learning techniques have been used for the development of novel drug candidates, with the methods for designing drug targets and novel drug discovery now routinely combining machine learning and deep learning algorithms to enhance the efficiency, efficacy, and quality of developed outputs. (11)

2.1 Supervised Learning Approaches

Supervised learning methods require labeled training datasets where the relationship between input features and desired outputs is explicitly provided. Machine learning algorithms including Random Forest and Decision Trees predict drug-target interactions and aid in virtual screening, support vector machines classify leads on bioactivity data, neural networks model QSAR to optimize lead compounds, and K-means clustering groups compounds with similar chemical properties aiding compound selection. (12) The generation and incorporation of big data through technologies such as high-throughput screening and high-throughput computational analysis of databases used for both lead and target discovery has increased the reliability of machine learning and deep learning incorporated techniques. (13)

2.2 Unsupervised Learning and Network Approaches

Graph machine learning is receiving growing interest within the pharmaceutical and biotechnology industries for its ability to model biomolecular structures, the functional relationships between them, and integrate multi-omic datasets amongst other data types, with key milestones including repurposed drugs entering in vivo studies suggesting graph machine learning will become a modelling framework of choice within biomedical machine learning. (14) Network-based approaches leverage biological relationships encoded in protein–protein interaction

networks, drug–gene networks, and disease pathways to identify novel associations and therapeutic opportunities.

2.3 Deep Learning Architectures

Machine learning and deep learning models support cancer phenotyping, including tumor detection, molecular subtyping, prognosis, and treatment response prediction across histopathology, radiology, and multi-omics data, with AI-enabled virtual screening, drug repurposing, generative molecular design, and hybrid computational–experimental pipelines streamlining oncology drug discovery and optimization. (15) Deep learning methods employ artificial neural networks with multiple layers to automatically learn hierarchical feature representations. Artificial intelligence is rapidly reshaping cancer research and personalized clinical care, with availability of high-dimensionality datasets coupled with advances in high-performance computing and innovative deep learning architectures leading to an explosion of AI use in various aspects of oncology research ranging from detection and classification of cancer to molecular characterization of tumors and their microenvironment to drug discovery and repurposing to predicting treatment outcomes for patients. (16) Convolutional neural networks (CNNs) excel at processing spatial data such as medical images, while recurrent neural networks (RNNs) and long short-term memory (LSTM) networks handle sequential biological data. Deep learning-based models for drug-target interactions prediction utilizing long short-term memory neural networks have shown improvement in DTI prediction performance, with proteins' evolutionary features extracted via Position Specific Scoring Matrix and Legendre Moment associated with drugs' molecular substructure fingerprints to form feature vectors of drug-target pairs. (17)

3. Artificial Intelligence-Based Drug Repurposing in Cancer

3.1 Concept and Strategic Advantages

Drug repurposing involves identifying the drug, evaluating its efficiency using preclinical models, and proceeding to phase II clinical trials, with identification of drug candidates made through

computational and experimental approaches utilizing public databases for drugs, data from primary and translational research, clinical trials, anecdotal reports regarding off-label uses, and other published human data information. (18) Drug repurposing has emerged as a powerful, cost-effective strategy for therapeutic innovation amid increasing global disease burdens and the limitations of traditional drug development, which is time-consuming, costly, and marked by high failure rates, with repurposed drugs such as thalidomide, sildenafil, metformin, and minoxidil demonstrating clinical potential. (19)

3.2 Machine Learning-Based Repurposing Strategies

In silico drug target prediction provides valuable information for drug repurposing, understanding of side effects as well as expansion of the druggable genome, with the development of robust methods for drug target prediction by leveraging class imbalance-tolerant machine learning frameworks with novel training schemes that incorporate drug-gene phenotype similarity and gene expression profile similarity to uncover novel opportunities of drug repurposing that may benefit cancer treatment. (20) Target repositioning, a strategy which relies on the repurposing of known targets for new diseases, leading to new treatments, less side effects and potential drug synergies, uses biological networks that have emerged as powerful tools for integrating heterogeneous data and facilitating the prediction of biological or therapeutic properties, and are widely employed to predict new therapeutic targets by characterizing potential candidates based on their interactions within a protein-protein interaction network. (21)

3.3 Drug–Target Interaction Prediction and Network Approaches

Phosphodiesterase-5 inhibitors, used clinically for erectile dysfunction and pulmonary arterial hypertension, have shown therapeutic capacity as repurposed drugs in oncology with emerging evidence suggesting their role in enhancing anti-tumor immune response by mediating various immune cells, with artificial intelligence as a new approach composed of traditional machine learning and deep learning methods potentially used to identify

targets of immune cells and predict efficacy for repurposed drugs toward malignancies. (22) Graph neural network-based models predict drug synergy using molecular structure and gene expression data from cancer cell lines, with drugs represented as molecular graphs and processed through GATv2 layers to capture structural relationships and cell lines encoded via attention-based embeddings of landmark genes, and when trained on large datasets and benchmarked against classical machine learning models, consistently outperforming all baselines with gains in AUPR and AUC while maintaining strong performance in generalization tasks involving unseen drugs and cell lines. (23)

4. AI in Cancer Target Discovery

4.1 Genomic and Transcriptomic Analysis

Artificial intelligence increasingly enables integrative analysis of complex biomedical data to identify actionable therapeutic vulnerabilities, with AI advancing mechanistic cancer target discovery through processing of large-scale genomics, transcriptomics, proteomics, metabolomics, single-cell profiling, spatial and clinical datasets using machine learning and deep learning algorithms to identify candidate biomarkers, driver genes, dysregulated pathways, tumor dependencies, and molecular targets that traditional methods often miss. (24) Machine learning emerged as a powerful tool in pharmaceutical research offering data-driven insights and accelerating lead identification for drug discovery, with machine learning-assisted virtual screening strategies successfully preselecting compounds with potential inhibitory activity from vast libraries, highlighting the value of machine learning approaches in advancing personalized and targeted therapies for cancer treatment. (25)

4.2 Biomarker Discovery and Patient Stratification

Machine learning plays a critical role in changing the cancer drug development landscape by addressing the problem of tumour heterogeneity and enabling the discovery and development of cancer biomarkers and clinical trial design, with the scarcity of clinical patient data and the current focus on genetic aberrations as primary drug targets limiting the

performance of anticancer drug repurposing approaches that rely solely on genomics-based information. (26) Artificial intelligence in biomarker discovery improves precision medicine by uncovering biomarker signatures essential for early detection and treatment of diseases within vast and diverse datasets, with deep learning and machine learning diagnostics representing transformative technologies changing how biomarkers are made by finding patterns in large datasets and enabling accurate and effective therapies. (27) The rapid advancement of high-throughput technologies, particularly next-generation sequencing, has revolutionized cancer research by enabling investigation of genetic variations and elevated the significance of precision oncology, with bioinformatics tools including tools for data structuring, pathway analysis, network analysis, and tools for analyzing biomarker signatures significantly impacting cancer research by uncovering novel biomarkers, driver mutations, oncogenic pathways, and therapeutic targets. (28)

4.3 Multi-Omics Integration for Target Identification

The integration of multi-omics data spanning genomics, transcriptomics, proteomics, metabolomics and radiomics can improve diagnostic and prognostic accuracy when accompanied by rigorous preprocessing and external validation, with artificial intelligence particularly deep learning and machine learning bridging the gap by enabling scalable non-linear integration of disparate omics layers into clinically actionable insights through cutting-edge AI methodologies including graph neural networks for biological network modeling and transformers for cross-modal fusion. (29) Multiomics data integration approaches offer comprehensive functional understanding of biological systems with significant applications in disease therapeutics, with AI-driven bioinformatics playing a crucial role in multiomics by computing scores to prioritize available drugs and assisting clinicians in selecting optimal treatments, while AI-driven bioinformatics plays a crucial role in identifying molecular targets for innovative drug development or the repurposing of existing therapies. (30)

5. Role of Deep Learning in Molecular and Drug Interaction Prediction

5.1 Drug–Target Affinity Prediction Models

Drug-target interaction prediction plays a vital role in drug discovery, with deep learning approaches having emerged as powerful and efficient tools for predicting DTIs, encompassing feature representation strategies for drugs and proteins followed by examination of various deep learning architectures including deep neural networks, recurrent neural networks, convolutional neural networks, graph neural networks, and transformer-based models with applications in drug repositioning, drug design, and precision medicine. (31) Drug-target interaction and affinity prediction using deep learning models has been presented to overcome the challenges of interaction prediction through precise and efficient end results, with deep learning models having addressed the limitations of traditional methods particularly in capturing complex relationships between drugs and their targets. (32)

5.2 Graph Neural Network Approaches

Graph neural networks have been introduced for drug-target affinity prediction by utilizing the structural information of molecules and proteins through building graphs of drug molecules and proteins respectively, with graph neural networks obtaining their representations and methods proposed for drug-target affinity prediction showing strong robustness and generalizability. (33) A novel deep-learning-based prediction model based on graph convolutional neural networks for protein-ligand binding affinity reduces the computational time and resources normally required by traditional convolutional neural network models, with graph convolutional neural networks representing protein-ligand complex structures as graphs of multiple adjacency matrices whose entries are affected by distances and feature matrices describing molecular properties. (34) An intermolecular graph transformer approach that employs a dedicated attention mechanism to model intermolecular information with a three-way transformer-based architecture outperforms state-of-the-art approaches by substantial margins for binding activity and binding pose prediction and exhibits

superior generalization ability to unseen receptor proteins than state-of-the-art approaches. (35)

5.3 Advanced Architectures and Transformer Models

A novel deep learning framework combining transformer and graph neural networks for predicting drug-target interactions utilizes graph convolutional neural networks to capture global and local structure information of drugs and convolutional neural networks to capture sequence features of targets, with multi-layer transformer encoders integrating features and generating final representations that outperform previous graph-based and transformer-based methods. (36) Deep learning has emerged as a promising approach to advance drug discovery by accurately predicting interactions between proteins and small molecules or ligands, with deep learning-based tools leveraging convolutional and graph neural networks to capture the complex three-dimensional nature of interactions and demonstrating significant improvement in predictive reliability outperforming conventional techniques and recent machine learning models. (37) Evidential deep learning for uncertainty quantification in neural network-based drug-target interaction prediction integrates multiple data dimensions including drug 2D topological graphs and 3D spatial structures and target sequence features, providing uncertainty estimates for predictions through a novel EviDTI approach that demonstrates competitiveness against baseline models and provides well-calibrated uncertainty information enhancing efficiency of drug discovery. (38)

6. Applications of AI in Different Cancer Types

6.1 Non-Small Cell Lung Cancer

Machine learning-assisted virtual screening for non-small cell lung cancer targeting the Platelet-Derived Growth Factor Receptor has successfully preselected compounds with potential PDGFRA inhibitory activity from vast libraries of 1.048 million compounds, with the approach validating candidates through traditional genetic algorithm-based virtual screening and docking methods and molecular dynamic simulations. (25)

6.2 Breast Cancer and Triple-Negative Disease

A machine learning-driven virtual screening pipeline for triple-negative breast cancer identified potent dual IDO1 and TDO inhibitors using an in-house machine learning classification model developed with IC50 values, with the eXtreme Gradient Boosting with Random Forest classifier achieving the highest performance and molecular docking and molecular dynamics simulations confirming stability of protein-ligand complexes. (39)

6.3 Prostate Cancer

A multi-layer network approach incorporating additional information such as gene regulation, metabolite interactions, metabolic pathways, and disease signatures was employed for target repositioning in prostate cancer, successfully predicting five novel promising therapeutic targets including IGF2R, C5AR, RAB7, SETD2 and NPBWR1 through training machine learning algorithms on features extracted from networks. (21)

6.4 Hematological Malignancies

Machine learning-enabled transomics analysis identified three therapeutic targets for MYC-driven diffuse large B cell lymphoma by leveraging a proprietary machine learning platform that unlocked functional drivers of disease to identify novel drug targets, with MYC-conditional cell lines and multiomics data including genomic, transcriptomic, proteomic, and phosphoproteomic information used to identify novel targets that reproduce MYC inactivation. (40)

6.5 Colorectal Cancer

A systematic comparison of Random Forest Classifier, deep learning, and graph neural network models including GAT, GCN, and MPNN for identifying COX-2 inhibitors in colorectal cancer demonstrated that both RFC and deep learning models outperformed GNN models, with the RFC model ultimately verified as the optimal model for activity screening of traditional Chinese medicine-derived compounds. (41)

6.6 Renal Cell Carcinoma

Deep learning and machine learning algorithms combined with single-cell transcriptome sequencing data successfully identified five ccRCC-specific compounds including two FDA-approved drugs and three novel compounds through analysis of tumor microenvironment characteristics and identification of key transcription factors. (42)

7. AI Integration with Precision Oncology

7.1 Personalized Treatment Selection and Companion Diagnostics

Recent advances in precision oncology have led to significant breakthroughs through targeting defined oncogenic drivers, with a paradigm shift toward multi-targeted, AI-enhanced strategies that harness high-throughput multi-omic data to inform rational design of combination therapies by leveraging artificial intelligence for drug discovery and repurposing, response prediction, and clinical trial optimization. (43) Multiple new trial designs including basket and umbrella trials, master platform trials, and N-of-1 patient-centric studies are beginning to supplant standard phase I, II, and III protocols, allowing for accelerated drug evaluation and approval and molecular-based individualized treatment, with real-world data and exploitation of digital apps and structured observational registries utilized in conjunction with machine learning and artificial intelligence to further accelerate knowledge acquisition. (44)

7.2 Multi-Omics Integration for Patient Stratification

AI and machine learning integration with patient-derived organoids enables scalable analysis of high-dimensional datasets including imaging, transcriptomics, proteomics, and pharmacological readouts to support prediction of drug sensitivity, biomarker discovery, and patient stratification, with recent advances such as deep learning, transfer learning, federated learning, and self-supervised learning enhancing phenotypic profiling and translational prediction. (45)

7.3 Clinical Decision Support Systems

Multimomics data including imaging radiomics and various types of molecular biomarkers have been increasingly investigated for better diagnosis and therapy in precision oncology, with artificial intelligence including machine learning and deep learning techniques combined with exponential growth of multimomics data having great potential to revolutionize cancer subtyping, risk stratification, prognostication, prediction and clinical decision-making. (46) Multi-omics integration implementing machine learning and deep learning approaches for data interpretation has yielded promising biomarker panels at single-molecule, multi-molecule, and cross-omics levels supporting cancer diagnosis, prognosis, and therapeutic decision-making, with cutting-edge advances in single-cell multi-omics and spatial multi-omics technologies expanding the scope of biomarker discovery and deepening understanding of tumor heterogeneity. (47)

8. Current Challenges and Limitations

8.1 Data Quality and Standardization

Artificial intelligence implication remains intricate for researchers and clinicians lacking specific training in computational tools and informatics, with data curation posing a significant challenge as different parameters, instruments, and sample preparation approaches are employed for generating big data sets. (3) In a systematic review of AI-augmented genomic biomarker identification studies from the 39 reviewed studies, only 22.5 percent conducted external validation, 7.5 percent included prospective cohorts, and fewer than 20 percent addressed regulatory alignment, with only 25 percent reporting open-source code availability limiting reproducibility. (48)

8.2 Model Interpretability and Explainability

Cross-cutting limitations in AI for precision oncology are examined including data quality and representativeness, class imbalance, bias and fairness, model interpretability, and ethical, privacy, and regulatory challenges in clinical deployment. (15) The rapid proliferation of deep learning-driven docking methods has created uncharted challenges in translating *in silico* predictions to biomedical reality, with deep learning docking methods exhibiting high steric tolerance and most methods exhibiting

significant challenges in generalization particularly when encountering novel protein binding pockets. (49)

8.3 Clinical Translation Barriers

Clinical utility of predictive models faces significant translational bottlenecks such as algorithmic interpretability, data heterogeneity, and the integration of these pipelines into routine clinical workflows, with research highlighting transformative potential of predictive genomics while outlining persistent challenges that must be overcome to realize full promise of personalized cancer medicine. (50)

8.4 Regulatory and Ethical Considerations

More than 60 AI-equipped medical devices have already been approved by the Food and Drug Administration in the United States, with active introduction of AI technology considered an inevitable trend in future medicine, though precision medicine based on genome information faces challenges in clinical implementation. (51) The full potential of AI in drug discovery can only be realized with sufficient ground truth and appropriate human intervention at later pipeline stages, with the scientific community needing to carefully vet known information to address the reproducibility crisis. (4)

FUTURE PERSPECTIVES

9.1 Generative AI and De Novo Drug Design

Drug discovery and development remains complex and time-consuming, often hindered by high costs and low success rates, with artificial intelligence having emerged as a promising tool to accelerate and optimize these processes particularly in oncology by exploring application of AI-based methods for drug repurposing and natural product-inspired drug design in cancer focusing on potential to address challenges and limitations of traditional drug discovery approaches. (52)

9.2 Foundation Models and Large Language Models

Recent developments indicate that large language models trained on biomedical literature and protein

sequences could augment traditional ML approaches for oncology drug discovery. Large language models are proving their value in the pharmaceutical industry for tasks like drug design, repurposing, optimization and especially drug-target interaction prediction, with integration of large language models and graph neural networks in a contrastive learning setup predicting protein-protein interactions and achieving high precision in predicting binding affinities, sites, and interactions. (53)

9.3 Explainable AI and Trustworthy Implementation

Primary development target areas for AI-based therapeutics include federated learning for data privacy, explainable artificial intelligence for regulatory transparency, and quantum machine learning for molecular-scale optimization, charting the course to patient-specific, scalable neuro-oncology nanomedicine through convergence of computational modeling, intelligent materials, and advanced imaging modalities. (54)

9.4 Real-World Data Integration and Adaptive Platforms

The application of artificial intelligence in medicine particularly through machine learning marked significant progression in drug discovery, with artificial intelligence acting as powerful catalyst in narrowing gap between disease understanding and identification of potential therapeutic agents, highlighting importance of data quality, algorithm training, and ethical considerations especially in-patient data handling during clinical trials. (55)

CONCLUSION

This comprehensive review demonstrates that artificial intelligence has fundamentally transformed the landscape of oncology drug discovery and target identification. Artificial intelligence is rapidly reshaping cancer research and personalized clinical care, with availability of high-dimensionality datasets coupled with advances in high-performance computing and innovative deep learning architectures leading to an explosion of artificial intelligence use in various aspects of oncology research from detection and classification of cancer to molecular

characterization of tumors and their microenvironment to drug discovery and repurposing to predicting treatment outcomes for patients. (16) The integration of artificial intelligence into cancer treatment represents a major advancement in diagnostic, prognostic, and therapeutic methods, with artificial intelligence accelerating drug discovery by identifying novel compounds, optimizing dosages, and repurposing existing drugs thereby enhancing treatment development. (56) AI-enabled drug repurposing and target discovery offer compelling advantages: substantially reduced development timelines, decreased attrition rates, lower costs, and improved prediction accuracy compared to traditional methods. Artificial intelligence is transforming drug discovery by enabling rapid identification of existing drugs with potential anti-cancer properties through drug repurposing, offering cost-effective and time-efficient alternatives to traditional drug development particularly in oncology where the need for novel therapies is urgent. (1) However, realizing AI's full potential in precision oncology requires addressing critical challenges. Emerging directions such as multimodal foundation models, federated learning, artificial intelligence stewardship, and patient-specific digital twins signal a paradigm shift toward dynamic personalized cancer management, with realizing full potential of artificial intelligence requiring rigorous validation, transparent reporting, and close collaboration between clinicians, data scientists, regulators, and patients to ensure equitable patient-centered benefit. (15) Artificial intelligence applications in drug discovery, target identification and drug repurposing for cancer highlight that AI-driven algorithms are used to predict drug responses and identify novel therapeutic targets, with case studies illustrating successful applications and future directions exploring emerging trends and potential advancements in AI-driven cancer research. (57) Future success depends on standardized data practices, prospective clinical validation, transparent algorithmic design, ethical oversight, and genuine integration of AI-driven insights into routine oncology workflows. When coupled with rigorous experimental validation and clinical evidence generation, AI represents a transformative frontier promising to accelerate the delivery of life-saving cancer therapeutics.

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