Artificial intelligence for Glioblastoma drug discovery

J.Sales-Llopis

Neurosurgery Department, General University Hospital Alicante, Spain

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- Artificial Intelligence in Glioblastoma-Transforming Diagnosis and Treatment
- GCN-BBB: Deep Learning Blood-Brain Barrier (BBB) Permeability PharmacoAnalytics with Graph Convolutional Neural (GCN) Network
- Effective targeting of PDGFRA-altered high-grade glioma with avapritinib
- Artificial Intelligence-Assisted Drug and Biomarker Discovery for Glioblastoma: A Scoping Review of the Literature
- Discovery of key molecular signatures for diagnosis and therapies of glioblastoma by combining supervised and unsupervised learning approaches
- Integrated regulatory and metabolic networks of the tumor microenvironment for therapeutic target prioritization
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- Identification of a Novel Eight-Gene Risk Model for Predicting Survival in Glioblastoma: A Comprehensive Bioinformatic Analysis

see Artificial intelligence for drug discovery

Artificial intelligence (AI) has emerged as a transformative tool in healthcare, particularly in drug and biomarker discovery, where it can enhance precision, streamline discovery processes, and optimize treatment strategies. Despite its potential, the application of AI in glioblastoma (GB) research, especially in identifying novel biomarkers and therapeutic targets, remains underexplored.

Artificial intelligence (AI) is significantly advancing glioblastoma (GBM) drug discovery by identifying novel therapeutic targets, predicting treatment responses, and optimizing clinical trial designs. Here are some notable AI-powered tools and drug candidates in GBM research:

AI-Powered Tools for GBM Research

1. **PandaOmics by Insilico Medicine**: This AI-driven platform integrates multi-omics data to identify potential therapeutic targets for diseases, including GBM. A study utilizing PandaOmics identified dual-purpose therapeutic targets implicated in both aging and GBM, showcasing its capability in uncovering novel targets for drug development. 😘cite😝turn0search1😛

2. **Deep Docking AI Platform**: Employed by Rakovina Therapeutics, this platform enables the rapid in silico screening of billions of compounds to identify promising small molecules for cancer therapy. Rakovina has advanced AI-derived drug candidates into preclinical validation, highlighting the platform's efficiency in accelerating drug discovery. 😘cite😝turn0search5😛

3. **i2Contour by MRIMath, LLC**: Supported by the National Cancer Institute, i2Contour is an AI-aided device that assists in measuring and labeling GBM during surgery. This tool provides an interpretable, physician-in-the-loop approach, enhancing surgical precision and potentially improving patient outcomes. 😙cite😆turn0search4😀

Artificial Intelligence Identified Drug Candidates for Glioblastoma

Artificial intelligence (AI) has significantly advanced the discovery of potential drug candidates for glioblastoma, an aggressive and often treatment-resistant brain tumor. By analyzing complex biological data, AI accelerates the identification of novel therapeutic targets and effective compounds.

AI-Driven Drug Discovery Initiatives:

Lantern Pharma's LP-184: Utilizing their AI platform, RADR®, Lantern Pharma has developed LP-184, a drug candidate that has received Fast Track Designation from the FDA for glioblastoma treatment. LP-184 is currently in Phase 1A clinical trials, showing promise in penetrating the blood-brain barrier and targeting tumor cells effectively.

USC's Gene Reprogramming Approach: Researchers at the University of Southern California employed AI to identify genes capable of transforming glioblastoma cells into dendritic cells. This innovative strategy aims to prompt the immune system to recognize and attack cancer cells, with preclinical studies in mice demonstrating a 75% increase in survival rates. KECK SCHOOL OF MEDICINE

Rakovina Therapeutics' PARP-1 Inhibitors: In collaboration with AI platforms, Rakovina Therapeutics has synthesized novel small-molecule drug candidates designed as PARP-1 selective inhibitors. These compounds are engineered to cross the blood-brain barrier, potentially offering new treatment avenues for glioblastoma and other brain cancers. BIOSPACE

TwoXAR and 1ST Biotherapeutics Collaboration: TwoXAR, an AI-driven drug discovery company, has partnered with 1ST Biotherapeutics to identify and develop new treatments for glioblastoma. Their AI platform analyzes vast datasets to pinpoint drug candidates that could slow or halt tumor progression. FIERCE BIOTECH

AI in Drug Repurposing and Biomarker Discovery:

AI has also been instrumental in repurposing existing drugs for glioblastoma treatment. A study highlighted the identification of oncology drugs, such as elesclomol, that target various aspects of glioma etiology. These findings suggest that AI can efficiently uncover new applications for established drugs, potentially expediting the availability of effective therapies. NATURE

Moreover, AI-assisted approaches have been employed to discover novel biomarkers and therapeutic targets for glioblastoma. By integrating multi-omics data and literature analysis, platforms like PandaOmics have predicted new age-associated targets, offering insights into personalized treatment strategies. PUBMED CENTRAL

In summary, AI is revolutionizing glioblastoma research by accelerating drug discovery, identifying novel therapeutic targets, and repurposing existing medications. These advancements hold promise for developing more effective treatments and improving patient outcomes in the fight against this

formidable cancer.

Reviews

A review aims to map the existing literature on AI-driven approaches for biomarker and drug discovery in GB, highlighting key trends and gaps in current research. Design: Following a PRISMA methodology, this scoping review examined studies published between 2012 and 2024. Searches were conducted across multiple databases, including MEDLINE (PubMed), Scopus, the Cochrane Library, and Web of Science (WOS). Eligible studies were screened, and relevant data were extracted and synthesized to provide a comprehensive overview of AI applications in GB research. Results: A total of 224 records were identified, including 210 from PubMed, 104 from Scopus, 4 from WOS, and 6 from the Cochrane Library. After screening and applying eligibility criteria, 33 studies were included in the final review. These studies showcased diverse AI methodologies applied to both drug discovery and biomarker identification, focusing on various aspects of GB biology and treatment. Conclusions: This scoping review reveals an increasing interest in AI-driven strategies for biomarker and drug discovery in GB, with promising initial results. However, further large-scale, rigorous studies are needed to validate real-world applications of AI and the development of standardized protocols to enhance reproducibility and clinical translation [1)].

Bioinformatics and computational biology studies

Identifying potential molecular signatures and associated drug molecules is crucial for the diagnosis and therapies of GBM. This study suggested GBM-causing ten key genes (ASPM, CCNB2, CDK1, AURKA, TOP2A, CHEK1, CDCA8, SMC4, MCM10, and RAD51AP1) from nine transcriptomics datasets by combining supervised and unsupervised learning results. Differential expression patterns of key genes (KGs) between GBM and control samples were verified by different independent databases. Gene regulatory network (GRN) detected some important transcriptional and post-transcriptional regulators for KGs. The KGs-set enrichment analysis unveiled some crucial GBM-causing molecular functions, biological processes, cellular components, and pathways. The DNA methylation analysis detected some hypo-methylated CpG sites that might stimulate the GBM development. From the immune infiltration analysis, we found that almost all KGs are associated with different immune cell infiltration levels. Finally, we recommended KGs-guided four repurposable drug molecules (Fluoxetine, Vatalanib, TGX221, and RO3306) against GBM through molecular docking, drug-likeness, ADMET analyses, and molecular dynamics simulation studies. Thus, the discoveries of this study could serve as valuable resources for wet lab experiments to take a proper treatment plan against GBM [2)].

1)
Conte L, Caruso G, Philip AK, Cucci F, De Nunzio G, Cascio D, Caffo M. Artificial Intelligence-Assisted Drug and Biomarker Discovery for Glioblastoma: A Scoping Review of the Literature. Cancers (Basel). 2025 Feb 7;17(4):571. doi: 10.3390/cancers17040571. PMID: 40002166.
2)
Sarker A, Aziz MA, Hossen MB, Mollah MMH, Al-Amin, Mollah MNH. Discovery of key molecular signatures for diagnosis and therapies of glioblastoma by combining supervised and unsupervised learning approaches. Sci Rep. 2024 Nov 11;14(1):27545. doi: 10.1038/s41598-024-79391-2. PMID: 39528802; PMCID: PMC11554889.