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A Systematic Review of AI-Driven Approaches for Biomarker Discovery and Drug Response Prediction in Precision Cancer Treatment

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Abstract

The field of AI has transformed precision oncology by providing new methods for discovering biomarkers and predicting how patients will respond to drugs.The applications proved essential for developing personalized treatment plans which addressed the intricate nature of cancer.The study collected data from research articles published between 2015 and 2025 which examined AI techniques that used genetic transcriptomic and proteomic information to enhance cancer diagnosis and treatment development and patient care.AI-driven approaches brought major progress in two areas through their work on finding useful biomarkers and their ability to predict how individual patients would respond to medications with deep learning (DL) models, such as convolutional artificial neural networks (CNNs) and recurrent artificial neural networks (RNNs) and graph-based artificial neural networks demonstrating better results with multi-omics data which includes different types of cancer data from breast cancer to lung cancer to colorectal cancer to glioblastoma cancer and other cancers.The challenges of data integration and interpretability and clinical implementation have persisted despite the progress made in this field.AI shows great potential to transform cancer treatment according to this review which presents methods for using multi-omics data together with solutions to ethical problems which will lead to better use of medical technology in healthcare.Information from credible research repositories such as PubMed,Scopus, IEEE Xplore, Google Scholar, Nature, and Web of Science were used.

Keywords: Artificial Intelligence, Precision Oncology, Biomarker Discovery, Drug Response Prediction, Personalized Medicine, Machine Learning, Deep Learning

1 Introduction

Cancer remains a foremost global health challenge, with over 10 million deaths annually and incidence rates continuing to rise Bray et al. (2024). The increasing global population, extended life expectancy, and contributing elements such as tobacco use, inadequate diet, and toxic exposure have substantially driven cancer prevalence Alum et al. (2024). However, developing nations bear an imbalanced load, accounting for nearly 70 percent of oncology-associated deaths. Some of the most commonly affected anatomical regions include the lungs, breast, liver, brain, and stomach cancer. Preventive measures, including quitting tobacco, immunization programs, and nutritional modifications, have shown the potential to substantially lower cancer incidence Ibiam et al. (2023). The integration of artificial intelligence (AI) into cancer treatment has revolutionized how cancer is diagnosed, indicated, and treated. The growing need for tailored medical solutions to treat individual patients drives this transformation.- Present-day treatment methods now include patient-specific genetic information together with their environmental factors and personal choices and all other vital aspects of their existence. The advances in AI-based methods are establishing new developments which will drive targeted cancer treatment research toward better accuracy in treatment evaluation and the creation of customized treatment plans.Farina et al. (2022).The applications play a crucial role in discovering operational objectives which complete their pharmaceutical development process for treating cancers with multiple different characteristics present in breast, lung, brain, and colorectal cancer cases. Machine learning and deep learning, as AI techniques, have shown exceptional capabilities to unify multiple omics data types while they improve diagnostic precision and patient treatment results. The systematic review examines AI-based methods which scientists use to discover biomarkers and predict drug responses in precision cancer therapy. The current study aims to achieve complete understanding of present research through study findings from recent studies while we demonstrate how artificial intelligence can transform healthcare and show which obstacles exist and what future research should pursue in medical settings.

Biomarker Discovery

The advanced algorithms of artificial intelligence enable researchers to analyze extensive genomic, transcriptomic, proteomic, and metabolomic datasets which leads to a significant change in traditional methods of discovering biomarkers. The AI models discover new connections within complex high-dimensional data which traditional statistical methods fail to identify unlike conventional theory-based approaches.Dai & Shen (2022).In the filed of AI the platforms like pandaOmics use bioinformatics methods to analyze complete omics data which helps researchers find essential treatment targets and biomarkers needed for cancer treatment.These platforms make use of high-throughput technologies to collect vast biological datasets as-

sembled over the past two decades Kamya et al. (2024). The research study demonstrates an explainable AI (XAI) deep learning model which detects biological indicators of non-small cell lung cancer (NSCLC) through its developed system. The study demonstrates the way interpretable models help to develop healthcare strategies which increase diagnostic accuracy while building trust among healthcare professionals toward artificial intelligence results.Dwivedi et al. (2023). Biomarker research relies on its ability to produce accurate biological measurements through its testing and analytical capabilities. The method assesses accuracy by measuring how closely results match actual biological measurements which require both sensitivity and specificity testing. Scientists need to maintain complete accuracy because it provides their research with trustworthy results that support their diagnostic and predictive work and treatment development. The artificial intelligence system enables scientists to use various 'omics' data types which include genomics and epigenomics and proteomics to study complex biological systems through their research on multi-layered biomarkers that lead to deeper insights into tumor biology. Researchers who use a complete research method will develop deep knowledge about cancer pathways and molecular processes which will help them develop better personalized treatments. The use of artificial intelligence for high-dimensional data processing and evaluation enables scientists to go beyond studying individual biomarkers which enables broader cancer biology research and helps advance precision medicine.

The incorporation of AI into biomarker research is predicted to greatly enhance the reliability of cancer detection. The diagnostic tests that use biomarkers as their basis demonstrate effectiveness but encounter challenges which lead to problems with their sensitivity and specificity performance. Sensitivity measures a biomarker's ability to correctly detect individuals with a disease (true positive rate), minimizing false negatives. Specificity evaluates a test's capacity to correctly determine which individuals do not have the medical condition (true negative rate) while decreasing instances of false identification. The two factors function as essential components which enable organizations to assess the diagnostic reliability of biomarkers. The common cancer detection techniques which include mammography for breast cancer and PSA testing for prostate cancer encounter problems because they produce incorrect positive and negative results which result in excessive testing or missed diagnostic opportunities.Das et al. (2024). AI automated methodologies have demonstrated exceptional capabilities to distinguish between cancer patients and healthy people which enables personalized healthcare and customized cancer treatments.*Bio-Marker Cancer Prediction System Using Artificial Intelligence* (2024).The development of next-generation sequencing (NGS) which works together with AI has enabled scientists to conduct precise cancer identification through improved biomarker discovery and cancer risk assessment methods.Dlamini et al. (2020).
AI visual data examination, which uses computational radiology and deep learning methods, collects substantial information from medical images that include CT scans and MRIs and

histopathological slides. The AI-computational biomarkers enable detection of cancer cell variability and identification of early malignancy indicators while showing hidden features that visual inspection cannot easily find.Koh et al. (2022).The biomarkers examine genetic and epigenetic and proteomic changes that occur in cancer. The machine learning algorithms process high-throughput data to detect DNA variations and classify different cancer types and predict how patients will respond to targeted treatment. Bhinder et al. (2021).Molecular biomarkers serve as crucial components for precision oncology because they enable medical professionals to develop personalized treatments which are based on the unique genomic characteristics of each tumor.Bhinder et al. (2021).

Drug Response Prediction

Oncology research uses drug response prediction to create personalized treatment methods for different types of cancer. The traditional methods of research depend on scientific studies which require extended time periods and extensive financial resources to complete. The latest advancements in Artificial Intelligence and machine learning technologies have transformed the process of drug discovery through the development of data-based computational systems that enhance both molecular target identification and drug creation processes.Zhavoronkov et al. (2019).AI helps to process the information in genomics, proteomics, and transcriptomics to reveal and validate new targets for drug discovery.Gawehn et al. (2016).Core scientific frameworks for the identification of key biomarkers and the research of potential drugs in clinical labs are in use in experimental data sets and cancer cell lines. The Broad institute Cancer Cell Line Encyclopedia (CCLE) database provides comprehensive multiomics data from over 1,000 cancer cell lines Wang et al. (2019). Oncology sensitivity Genomics, and The Cancer Genome Atlas (TCGA), Establish a basis for AI-driven drug screening. Research works incorporated in this review have implemented deep learning models, integrated algorithms, and graph-based neural networks to enhance drug sensitivity predictions throughout various cancers, including breast, emphasized personalized medicine modeling for breast cancer and discovered genomic markers for precision treatment and lung, colorectal, and glioblastoma showed that incorporating multi-omics data with deep learning substantially improves drug response prediction accuracy, highlighting the capability of AI-driven approaches in precision oncologySharifi-Noghabi et al. (2019). Discovered LXR agonists as glioblastoma inhibitorsChen et al. (2020), and discovered LSD-1 inhibitors for glioblastoma treatmentAlabed et al. (2022). These strategies not only enhancing therapy response predictions but also facilitate biomarker discovery and drug repurposing, enhancing the development of precision medicine in oncology.

Objectives

The objective of this systematic review was to evaluate the role of artificial intelligence (AI) in biomarker discovery and drug response prediction for precision cancer treatment. Specifically, the review aims to:

- The research investigates the capability of artificial intelligence methods together with machine learning and deep learning strategies to discover genetic markers and transcriptomic markers and proteomic markers and epigenetic markers. the effectivity of AI-driven models in predicting patient-specific responses to drugs combining multiple -omics data sources.
- Evaluate the effectivity of AI-driven models in predicting patient-specific responses to drugs combining multiple -omics data sources.
- The study of personalized oncology currently faces challenges which require scientists to determine future research paths and technology development needs for AI applications.

This objective establishes its field of study through its description which defines its main goal. The review process establishes specific scope and eligibility criteria which serve to define those who can participate in the study.

Methodology

This systematic review is conducted in compliance with the PRISMA framework. (www.prisma-statement.org)

Eligibility Criteria

Studies were included if they:

- Focused on AI methodologies for biomarker discovery or drug response prediction in cancer.
- Utilized genetic, transcriptomic, proteomic, or multi-omics datasets.
- Reported measurable outcomes such as biomarker identification, drug efficacy prediction, or clinical implementation.
- Were published in peer-reviewed journals between 2015 and 2025.

Studies were excluded if they:

- Did not involve AI methodologies.
- Focused on non-cancer diseases or non-human models.
- Were reviews, articles, or opinion pieces without primary data.

Search Methods and Search Strategy

Articles and reports shall be retrieved from electronic databases including PubMed, Scopus, IEEE Xplore, Web of Science, Google Scholar, and Nature databases. Essential data were retrieved, including research attributes, AI techniques, Machine Learning Approaches, data sources, Major Insight, and Medical significance. Studies were classified into biomarker discovery, drug response prediction, or combined, and AI performance was evaluated using precision, sensitivity, and specificity. All studies were organized using Mendeley and Excel. Repeated entries were eliminated, and full-text articles were reviewed without automation. Based on established eligibility rules selection process was performed at the title, abstract, and full-text levels.

The detailed search strings applied across each database are presented in Table 1. Each database required a tailored query to optimize retrieval while minimizing irrelevant results. PubMed queries were restricted to human studies and peer-reviewed journals, while Scopus and IEEE Xplore were targeted for clinical/preclinical data and oncology-specific AI methodologies respectively. Google Scholar and Nature queries focused on AI-based predictive studies, and Web of Science was used to capture multi-omics data integration studies.

Table 1: Search Strategy For Databases

Databases	**Search string**	**Objective**
PubMed (www.pubmed.ncbi.nlm.nih.gov)	((Cancer[Title/Abstract]) AND (Artificial Intelligence[Title/Abstract] OR machine learning[Title/Abstract] OR Deep Learning[Title/Abstract])) AND (Biomarker[Title/Abstract] OR Drug[Title/Abstract])	Focused on human studies and peer-reviewed journals

Databases	Search string	Objective
Scopus (www.scopus.com)	(TITLE-ABS-KEY(cancer) AND TITLE-ABS-KEY(artificial AND intelligence OR machine OR learning OR deep AND learning) AND TITLE-ABS-KEY(biomarker OR drug))	Included studies involving clinical and preclinical data
IEEE Xplore (www.ieeexplore.ieee.org)	”Artificial intelligence” OR ”Machine learning” OR ”Deep learning” AND ”Cancer” AND (”Biomarker” OR ”Drug”)	Limited to oncology-specific AI methodologies
Google Scholar (www.scholar.google.com)	allintitle: Cancer ”Artificial intelligence” OR ”machine learning” OR ”deep learning” Biomarker OR Drug	Included AI-based predictive studies in cancer
Nature (www.nature.com)	title:(”Cancer” AND (”Artificial intelligence” OR ”Machine learning” OR ”Deep learning”) AND (”Biomarker” OR ”Drug”))	Focused on AI applications in cancer research
Web of Science (www.webofscience.com)	(((TI=(Cancer)) AND TI=(Artificial intelligence OR machine learning OR deep learning)) AND TI=(Biomarker OR Drug)	Covered multi-omics data integration studies

Selection of study, Data Extraction

Data were extracted by independent investigators on genomics and transcriptomics, radiomics pathomics studies were classified based on the type of study(retrospective/prospective), data sources(Public database, Clinical trials, institution), (i) cancer type, (ii) number of patients, (iii) type of therapy, (iv) significant biomarkers, (v) feature selection methodology (if applicable), (vi) developed model, and (vii) achieved results.Multimodal data were defined as those

integrating three or more data modalities, while studies that combined only two modalities with real-world data (RWD) were not considered multimodal. The extracted information was reviewed to ensure accuracy and relevance.

Data analysis

Essential outcomes related to the strategies, AI-driven Approaches, and conclusions relevant to Biomarker Discovery and Drug prediction in precision cancer treatment are accurately arranged and interpreted. To provide an exhaustive understanding of current advancements and future directions, valuable insights like model performance, applicability, and trends are accurately reported.

Risk of Bias Assessment

The bias existed on the positives and negatives along the risk of bias of every study. The risk of bias was evaluated using the Cochrane bias assessment tool for randomized research and ROBINS-I for non-randomized research.In trying to inflate word count, consider the following example: Key domains under observation Kodell are as follows.

2 Results

A comprehensive search across multiple databases within the past 11 years produced a total of 1,998 results from PubMed, Google Scholar, Web of Science, Nature, IEEE Xplore, and Scopus. The process of eliminating duplicates resulted in the acquisition of 1,398 distinct results.Based on titles and abstracts, 500 relevant articles were identified and selected. Of these, 370 were excluded due to access restrictions (paid articles), and 83 were excluded as they were literature reviews and conference papers. At last, 47 research articles were included for full-text analysis. The complete selection process is illustrated in Figure 1 (PRISMA Workflow Diagram),which demonstrates the different steps used to identify studies and assess their screening results and eligibility criteria until their final inclusion.

The PRISMA workflow (Figure 1) begins with the identification phase, where 1,998 records were identified from six databases along with six registers. Before screening, 553 records were removed—comprising duplicates and records marked ineligible by automation tools. The screening process began with 1,398 records, which were evaluated through their titles and abstracts, but 898 records were removed from consideration at this point. The study started with 500 articles, but 370 articles were removed because they required paid access for viewing, which left 130 articles that were accessible to the public.A further 83 were excluded as litera-

ture reviews or conference papers. This resulted in 47 studies being included in the final review for full-text analysis.

This research investigated AI-driven biomarker discovery and drug response prediction throughout various cancers, such as breast cancer, lung cancer, colorectal cancer, brain cancer, liver cancer, stomach cancer, glioblastoma, gastric adenocarcinoma, and renal carcinoma. The evaluated research works implemented deep learning models (CNNs, RNNs, transformer-based models, MOLI, MM-DRP, Self-Supervised Learning), conventional machine learning methods (SVMs, Random Forests, Ensemble Learning, XGBoost, Decision Trees, Ridge Regression, LASSO), and network-based classification methods (Graph Neural Networks (GNNs), Network-Based Profiling).

The primary datasets used for learning algorithms and validation included GDSC, CCLE, TCGA, DrugBank, ChEMBL, BindingDB, UCSC Xena, CGGA, GEO, and clinical trial data (Checkmate 067, Keynote-189), which have been broadly applied in cancer research. Multimodal deep learning frameworks integrating genomic, transcriptomic, and proteomic data substantially enhanced drug response prediction. Feature selection techniques such as LASSO, Boruta, PCA, Recursive Feature Elimination (RFE), and SHAP-based explainability models were applied to refine biomarker identification.

Critical discoveries highlight that multi-omics dataset unification, graph neural networks, and AI-assisted feature filtering methods substantially enhance biomarker identification and drug sensitivity predictions. Studies identified lncRNA biomarkers (HCP5, USP30-AS1, PSMB8-AS1, AL133264.2, KIF20A) for glioblastoma prognosis and the role of PD-L1 in the prediction of the response to immunotherapy. LXR agonists were discovered as potential glioblastoma inhibitors, while LSD-1 inhibitors were identified for glioblastoma treatment. Self-supervised deep learning demonstrated efficacy in biomarker discovery from pathology slides, and network-based profiling methods improved drug response predictions by merging diverse biological datasets.

The field continues facing multiple challenges because of data heterogeneity and problems with interpretation and limits on clinical validation which exist despite the technological advancements.Upcoming studies should investigate explainable AI (XAI) together with practical healthcare assessment and AI-driven prediction integration to solve existing gaps between computational models and real-world oncology applications.

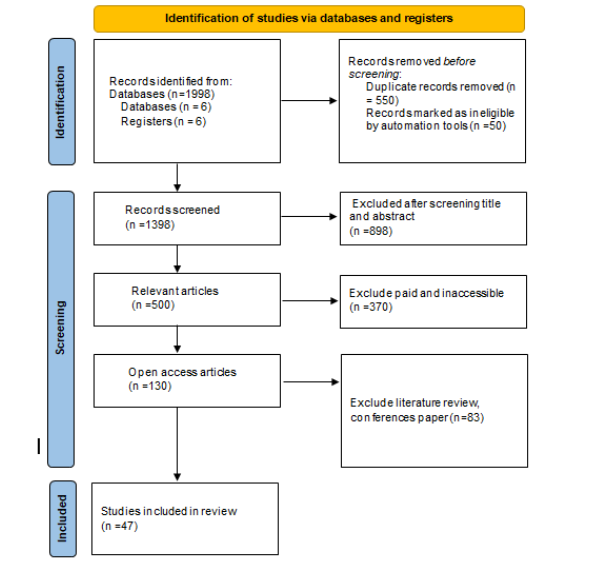

Figure 1: PRISMA WorkFlow Diagram

Table 2 below provides an overview of AI-driven research in biomarker discovery throughout multiple cancer types. The researchers used machine learning deep learning and network-based methods to evaluate multi-omics data which included genetic transcriptomic and proteomic biomarker information. The table provides a summary of key information which includes the study authors publication year type of cancer and specific biomarkers analyzed AI techniques applied datasets used validation approach and key findings. AI models showed improved accuracy for biomarker identification which led to better treatment response prediction. The researchers used multi-modal data integration and feature selection techniques to achieve better biomarker discovery results while maintaining essential clinical relevance. The findings showcase how AI systems help identify new biomarkers while improving precision oncology through their data-driven techniques.

Table 2: The review of the articles on Biomarker Discovery studies conducted on it

Author/Year of Publication	**Journal**	**Objective**	**Cancer type,Found Biomarker**	**Model Use**	**Dataset**	**Validation and performance**
Gao et al.Gao et al. (2021),2021	Frontiers in Genetics	Identifying lncRNA biomarkers for immune phenotype classification in Glioblastoma	Glioblastoma, HCP5,USP30-AS1, PSMB8-AS1, LINC01506,AL133264.2, LINC01684,	SsGSEA, ML, mRMR, RF	TCGA	Used TCGA transcriptome data to guide immunotherapy strategies
Suman and KulshresthaSuman & Kulshrestha (2024),2024	Human Genetics	Recognizing Gene Profiles and cell types in recurrent pediatric Glioblastoma using scRNA-Seq	Pediatric Glioblastoma,HMGB2, H2AFZ, HIST1H4C, KIAA0101, DUT	scRNA-Seq, ML, PCA, KNN, RF, XGBoost, DT	GEO	ML and scRNA-Seq helped classify gene signatures and cell types

Author/Year of Publication	Journal	Objective	Cancer type,Found Biomarker	Model Use	Dataset	Validation and performance
Han et al.Han et al. (2022),2022	Cancer Immunology, Immunotherapy	Evaluating the impact of DKK3 expression on prognosis and immunosuppression in Glioblastoma	Glio blastoma,DKK3	GSEA, ML	TCGA GBM	High DKK3 expression linked to poor prognosis, suggesting it as a therapeutic target
Han et al.Han et al. (2023),2023	Journal of Inflammation Research	Investigating the role of NOD1 in Glioblastoma prognosis and immunosuppression	Glio blastoma,NOD1	Bio informatics, ML, RF	TCG	High NOD1 expression linked to poor prognosis, highlighting it as a therapeutic target

Author/Year of Publication	Journal	Objective	Cancer type,Found Biomarker	Model Use	Dataset	Validation and performance
Ye et al.Ye et al. (2023),2023	Journal of Cancer Research and Clinical Oncology	Estimating glioma prognosis and effect to TMZ Therapy using a novel grading system	Glio blastoma,KIF20A	mRNA data analysis, ML, UC, PCA, Boruta	TCGA, CGGA, GEO	High NOD1 expression linked to poor prognosis, highlighting it as a therapeutic target
Niehues et al.Niehues et al. (2023),2023	Cell Reports Medicine	Generalizable biomarker prediction from cancer pathology slides using self-supervised deep learning	Various cancers ,Not specified	Self-supervised deep learning	Multi-centric dataset	Retro spective multi-centric study
Reck et al.Reck et al. (2021),2021	Annals of Oncology	Evaluating Pemetrexed plus platinum with/without pembrolizumab for NSCLC	NSCLC ,Not specified	Not specified	Clinical trial data	Protocol-specified final analysis from Keynote-189

Author/Year of Publication	**Journal**	**Objective**	**Cancer type,Found Biomarker**	**Model Use**	**Dataset**	**Validation and performance**
Rönnau et al.Rönnau et al. (2023),2023	Computational Methods and Programs in Biomedicine	Joint segmentation and quantification of nuclei NORs in AgNOR-stained images using CNN	Various cancers , Not specified	CNN-based approach	AgNOR-stained images dataset	Achieved reliable segmentation quantification
Sharifi-Noghabi et al.Sharifi-Noghabi et al. (2019),2019	Bioinformatics	Enhancing drug response prediction by fusing multi-omics datasets via deep learning models.This approach leverages diverse biological data to enhance predictive accuracy.	Various cancers ,Not specified	Deep neural networks (MOLI)	Multi-omics datasets	Improved drug response prediction accuracy

Author/Year of Publication	Journal	Objective	Cancer type,Found Biomarker	Model Use	Dataset	Validation and performance
Chiu et al.Chiu et al. (2019),2019	BMC Medical Genomics	Estimating tumor treatment efficacy using genomic data.	NSCLC , Not specified	Not specified	Clinical trial data	Protocol-specified final analysis from Keynote-189
Pagano et al.Pagano et al. (2025),2025	Life (MDPI)	To develop and validate an AI-based biomarker signature for predicting response to cytotoxic chemotherapy and targeted therapy	Metastatic Colorectal Cancer (mCRC), Not explicitly mentioned	Machine Learning	Genomic, Transcriptomic, and Clinical Data	Clinical validation planned

Author/Year of Publication	Journal	Objective	Cancer type,Found Biomarker	Model Use	Dataset	Validation and performance
Li et al.Li et al. (2019),2019	Scientific Reports	To identify potential biomarkers for gastric adenocarcinoma using bioinformatics analysis.	Gastric Adenocarcinoma ,FN1, SPARC, SERPINE1	Microarray and Bioinformatics	TCGA, GEO	The study utilized microarray and bioinformatics analyses to identify FN1, SPARC, and SERPINE1 as biomarkers associated with poor prognosis in gastric adenocarcinoma patients.

Author/Year of Publication	Journal	Objective	Cancer type,Found Biomarker	Model Use	Dataset	Validation and performance
Yang et al.Yang et al. (2024),2024	Front. Immunol.	Conducted a multi-omics analysis to identify disulfidptosis subtypes in glioblastoma, highlighting their implications for immunotherapy, targeted therapy, and chemotherapy.	Glioblastoma ,CD80, CD86, CTLA4, PDCD1, PDCD 1LG2, CD27,	SsGSEA, Transcriptomics, ML	TCGA, CGGA	Identified novel subtypes associated with immune response and therapeutic targets.
Huang et al.Huang et al. (2024),2024	Genes	Investigated the prognostic role of lncRNA NDUFA6-DT in gliomas, revealing its influence on immune modulation and synaptic transmission.	Gliomas, NDUFA6-DT	SsGSEA, RNAseq, ML (GLM, RF, Boruta, GBM, XGBoost, SVM-RFE)	UCSC Xena, TCGA, Ensembl, GEO, CGGA	Demonstrated significant correlation with glioma prognosis and immune response regulation.

Author/Year of Publication	Journal	Objective	Cancer type,Found Biomarker	Model Use	Dataset	Validation and performance
Joyce et al.Joyce et al. (2024),2024	Cancers	Identified serum proteins associated with CD133 using machine learning to predict 12-month survival in glioblastoma patients.	Glioblastoma, RPA2, AMPD2, DLK2, NEGR1, PDCL2, POLI, CEACAM3, ITGA6, PCDHGA10, SELENOW, IMM8A, CLN5	ML, Proteomics (LASSO, RFECV)	NIH	Developed a predictive model linking CD133-associated proteins to glioblastoma survival outcomes.
Bray F, Laversanne M, Sung H, Ferlay J, Siegel RL, Soerjomataram I, Jemal A.Bray et al. (2024),2024	CA: A Cancer Journal for Clinicians	To provide global estimates of cancer incidence and mortality for 36 cancers across 185 countries.	Various cancer types no specific biomarkers discussed.	Epidemiological analysis using GLOBOCAN database.	GLOBOCAN 2022 data.	Not applicable; descriptive statistics.

Table 3 below provides an overview of AI-driven research for drug response prediction. The research employed deep learning and reinforcement learning along with hybrid AI frameworks to assess treatment effectiveness and anticipate drug resistance patterns and enhance therapy selection. The table provides a summary of key information, including the study authors, publication year, Cancer type and specific AI techniques applied, datasets used, validation approach, and key findings. The AI models achieved better results in chemotherapy response prediction

when they used multiple biological datasets for analysis. The research study examined the need for actual clinical evaluations to verify whether AI-based drug sensitivity predictions align with medical decision processes and personalized treatment methods.

Table 3: An overview of the included Drug Response Prediction articles on the study

Author/Year of Publication	**Journal**	**Objective**	**Cancer type,Found Drug**	**Model Use**	**Dataset**	**Validation and performance**
Bomane et al. Bomane et al. (2019), 2019	Frontiers in Genetics	Predict paclitaxel response using DNA-methylation and miRNA data	Multiple Cancers, Paclitaxel	Multivariate Classifiers	TCGA, GEO	Accuracy: 92%
Bellmunt et al. Bellmunt et al. (2017), 2017	New England Journal of Medicine	Assess Pembrolizumab as second-line therapy	Urothelial Cancer, Pembrolizumab	Clinical Study with AI Analysis	Clinical Trial Data	Overall Survival Improved
Chiu et al. Chiu et al. (2019), 2019	BMC Medical Genomics	Predict tumor drug response using genomic data	Multiple Cancers, Multiple drugs	Deep Neural Networks	TCGA, GEO	AUC: 0.92
Chen et al. Chen et al. (2020), 2020	Eur. J. Med. Chem.	Discovery of LXR agonists as GB inhibitors	Glioblastoma, LXR agonists	SVM, NB	ChEMBL, BindingDB	In vivo testing on GB xenograft models showed tumor inhibition

Author/Year of Publication	Journal	Objective	Cancer type,Found Drug	Model Use	Dataset	Validation and performance
Neves et al. Neves et al. (2020), 2020	Eur. J. Med. Chem.	ML-based identification of anti-glioma lead compounds	Glioblastoma, 4m 4n compounds	SVM, RF, DNN	ChEMBL	In vitro and in vivo validation, reduced glioma growth in mice
Alabed et al. Alabed et al. (2022), 2022	RSC Adv.	Discovery of potent LSD-1 inhibitors using ML and molecular modeling	Glioblastoma, LSD-1 inhibitors	RF, XGBoost	ChEMBL	Tested in GB cells
Davis and Patel Davis & Patel (2019), 2019	J Immunother Cancer	PD-L1 as a predictive biomarker in FDA-approved immune checkpoint inhibitors	Multiple Cancers, Multiple immune checkpoint inhibitors	Clinical AI-based analysis	FDA approvals	Not specified
Escudier et al. Escudier et al. (2017), 2017	European Urology	Compare Nivolumab vs. Everolimus for renal carcinoma	Renal Cell Carcinoma, Nivolumab, Everolimus	AI-assisted Clinical Trial	Clinical Trial Data	Improved progression-free survival

Author/Year of Publication	**Journal**	**Objective**	**Cancer type,Found Drug**	**Model Use**	**Dataset**	**Validation and performance**
Hodi et al. Hodi et al. (2018), 2018	Lancet Oncology	Compare Nivolumab + Ipilimumab vs Monotherapies	Melanoma, Nivolumab, Ipilimumab	Clinical Trial AI-based analysis	Clinical Trial Data (Checkmate 067)	4-year survival benefit
Dong et al. Dong et al. (2015), 2015	BMC Cancer	Predict drug sensitivity using gene expression	Multiple Cancers, Multiple anticancer drugs	Recursive Feature Selection	TCGA, GEO	Accuracy: 88%
Hassan et al. Hassan et al. (2025), 2025	Frontiers in Oncology	Systematic review assessing AI's role in chemotherapy development, cancer diagnosis, and treatment	Various cancers, Not specified	AI-driven predictive models	Multiple oncology datasets	Evaluated AI's efficacy in predicting treatment responses
Ha et al. Ha et al. (2025), 2025	BMC Research Notes	Evaluate regression models for drug response prediction	Multiple cancer types, Multiple anticancer drugs	Ridge, LASSO, RF, XGBoost, SVR	GDSC	Performance metrics (R^2, RMSE) compared for 13 models

Author/Year of Publication	Journal	Objective	Cancer type,Found Drug	Model Use	Dataset	Validation and performance
Taj and Stein Taj & Stein (2022), 2022	Bioinformatics Advances	Drug response prediction and biomarker discovery using multimodal deep learning	Multiple cancer types	Multimodal deep learning model (MM-DRP)	Multiple genomic and drug response datasets	Model performance evaluated using cross-validation and independent test sets
Guo et al. Guo et al. (2023), 2023	Bioinformatics	DrDimont: explainable drug response prediction from differential omics data	Various cancers, Not specified	DrDimont	CCLE, GDSC	Provided explainable predictions with significant correlation to ground truth
Pak et al. Pak et al. (2023), 2023	Briefings in Bioinformatics	Improving drug response prediction by integrating multiple data sources using network-based profiling	Various cancers, Not specified	Network-based profiling	GDSC, CCLE	Enhanced prediction performance compared to single-data-source models

Author/Year of Publication	Journal	Objective	Cancer type,Found Drug	Model Use	Dataset	Validation and performance
Li et al. Li, Guo, Gao & Wang (2023), 2023	Bioinformatics	Enhancing cancer drug response prediction with multi-omics and morphology images contrastive representation learning	Various cancers, Not specified	MMCL-CDR	GDSC, CCLE	Improved prediction accuracy over existing methods

3 Discussion

AI applications in biomarker research and drug response prediction have reached new levels which now enhance precision oncology. The review demonstrates that deep learning and machine learning methods have become essential tools for detecting cancer biomarkers and choosing appropriate treatments.

AI models have developed methods to identify genomic and proteomic and epigenetic biomarkers which improve the ability to diagnose medical conditions and predict patient outcomes and assess treatment effectiveness. Multi-omic dataset integration enables researchers to validate biomarkers through more extensive processes which enhance both validation accuracy and clinical value of their findings. The development of new AI methods has increased accuracy in predicting biomarkers which researchers use to study tumor microenvironments and immune system biomarkers.

AI systems have been used in drug response prediction to create customized treatment methods and improve treatment results. The different computational techniques which researchers developed provide strong capabilities to forecast how patients will react to chemotherapy and their ability to withstand medication treatment. Advanced AI systems have demonstrated their effectiveness by detecting drug resistance pathways which improve treatment classification accuracy. Real-world clinical datasets which researchers analyzed

established a connection between computational modeling and clinical practice because they demonstrated how AI-based drug response predictions function in actual oncology environments.

The new developments have established their capabilities yet face critical challenges which still exist. Data heterogeneity continues to be a substantial limitation, as differences in multi-omics profiles diagnostic techniques and clinical datasets create inconsistencies which affect the functionality of AI models. The absence of uniform data processing pipelines and feature selection techniques further contributes to inconsistencies in forecasted results. The deep learning model complexity makes it difficult to understand their functions which creates problems for using them in clinical decision-making processes.

Current research depends on historical datasets, which creates a requirement for clinical trials that test AI predictions to establish their real-world effectiveness.Upcoming developments in this field should focus on integrating multiple biological data sources to improve biomarker exploration and drug response prediction precision.The adoption of secure AI models will enable organizations to work together across multiple institutions while protecting their data and meeting all regulatory requirements.

The implementation of AI techniques that improve model interpretability will help increase both the reliability and acceptance of AI systems used in cancer treatment. The successful deployment of AI predictive models in healthcare settings needs a rigorous evaluation process which will assess the ethical implications while checking compliance with oncology detection laws and outcome prediction rules and precision medicine regulations.

4 Conclusion

Artificial intelligence (AI) implementation has created fundamental transformations in both biomarker discovery and drug response prediction processes used in oncological research.The combination of multi-omics data and advanced AI methodologies leads to better drug prediction and biomarker identification through AI-driven models and machine learning techniques. The research in this review uses multi-omics datasets to develop better treatment methods which will transform cancer treatment through precise diagnosis and customized treatment plans that result in improved patient results. The process of converting research advances into medical practice needs to solve three main problems which include data integration and model interpretation and clinical application of the research results.The model depends on these three challenges which must be resolved to establish dependable performance standards.The expanding use of AI in support of personalized cancer treatment will create new medical practices for oncology which will develop into a new treatment period.The research program should establish research objectives that focus on developing AI methods which will enhance data collection through different sources and use AI systems for clinical operations.The ongoing development

of AI technology has the potential to bring major changes to personalized medicine while it strengthens drug discovery processes and improves cancer treatment methods.

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Glossary of Terms:

AI	Artificial Intelligence
ML	Machine Learning
DL	Deep Learning
CNN	Convolutional Neural Networks
RNN	Recurrent Neural Networks
GNN	Graph Neural Networks
SVM	Support Vector Machine
XGBoost	Extreme Gradient Boosting
RF	Random Forest
LASSO	Least Absolute Shrinkage and Selection Operator
TCGA	The Cancer Genome Atlas
GDSC	Genomics of Drug Sensitivity in Cancer
CCLE	Cancer Cell Line Encyclopedia
AUC	Area Under Curve
PCA	Principal Component Analysis
ROC	Receiver Operating Characteristic
PLMs	Protein Language Models
XAI	Explainable AI
AE	Autoencoders
VAE	Variational Autoencoders
RL	Reinforcement Learning
SHAP	Shapley Additive Explanations
BORUTA	Feature Selection Algorithm
scRNA-seq	Single-cell RNA Sequencing
HR	Hazard Ratio
C-index	Concordance Index
GEO	Gene Expression Omnibus
ChEMBL	Chemical Database
FDA	Food and Drug Administration
Federated Learning	Privacy-preserving collaborative AI