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Original Research Article

Ai-Driven Predictive Modeling for Identifying Personalized Therapeutic Targets in Oral Squamous Cell Carcinoma Using Molecular Profiling Data

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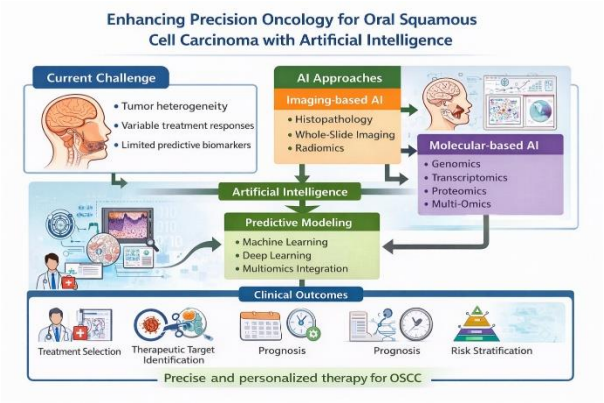
Abstract: ***Background***: Oral squamous cell carcinoma remains a major global health burden with limited improvement in outcomes despite advances in conventional treatment modalities. Objective: To systematically review and synthesize evidence on the application of artificial intelligence-based predictive models for identifying personalized therapeutic targets in oral squamous cell carcinoma, with a comparative focus on imaging-based and molecular-based approaches. Methods: A systematic review was conducted in accordance with PRISMA guidelines. Electronic databases, including PubMed/MEDLINE, Scopus, Web of Science, and Embase, were searched for relevant studies published between 2020 and 2025. Eligible studies applied artificial intelligence or machine learning techniques to imaging, molecular, or multimodal data in patients with oral squamous cell carcinoma. Results: Fourteen studies were included in the final analysis. Imaging-based artificial intelligence models demonstrated consistently high predictive performance, with reported area under the curve values ranging from approximately 0.85 to 0.95 across histopathological and radiological applications. Molecular-based artificial intelligence models showed wider variability, with area under the curve or C-index values ranging from approximately 0.75 to 0.90, reflecting underlying biological heterogeneity and differences in molecular platforms. Multimodal artificial intelligence models integrating imaging, molecular, and clinical data achieved superior performance, with area under the curve values frequently exceeding 0.90. Conclusion: Artificial intelligence–driven predictive modelling offers significant potential to advance precision oncology in oral squamous cell carcinoma. Imaging-based and molecular-based artificial intelligence approaches serve complementary roles, and integrated multimodal frameworks are likely to provide the greatest clinical benefit.

Keywords: Artificial intelligence, Oral squamous cell carcinoma (OSCC), Tumors, Patients, Imaging-based.

INTRODUCTION

Oral squamous cell carcinoma (OSCC) constitutes the predominant histological subtype of oral malignancies and remains a major contributor to cancer-related morbidity and mortality worldwide [1]. Despite advances in surgical techniques, radiotherapy delivery, and systemic treatment modalities, survival outcomes for OSCC have improved only modestly over recent decades [2]. Late-stage presentation, early regional metastasis, and frequent treatment resistance continue to limit therapeutic success. These challenges reflect not only delayed diagnosis but also the intrinsic biological complexity of OSCC, which is inadequately addressed by conventional treatment stratification strategies. OSCC is characterized by marked inter- and intra-tumoral heterogeneity, driven by diverse genetic, epigenetic, and transcriptional alterations [3]. Neoplasms with the same clinical stage

and histopathological grade are often heterogeneous in their molecular makeup, resulting in different rates of disease progression and response to available therapies [4]. While traditional clinicopathological parameters and staging criteria are crucial to the process of prognostication, they do not take this molecular diversity into account [5]. Therefore, treatment approaches based only on the anatomical and histological features of the disease can have a negative impact, and therefore substantiate the necessity for treatment strategies to be molecularly based and individualized. Oral squamous cell carcinomas (OSCCs) are the most common form of oral cancer and account for about 90% of all oral malignancies and constitute a significant proportion of head and neck cancer. OSCC remains a significant and troubling public health problem, particularly in populations where tobacco and alcohol are commonly used [6-10]. Patients with OSCC, even after considerable investments into diagnostic and therapeutic advancements, continue to have a poor prognosis as a result of the disease's high rates of metastasis, recurrence, and treatment response. Due to late-stage disease at diagnosis, the five-year survival rate for OSCC patients has plateaued between 50 to 60%, and this calls for enhanced innovation in reliable and robust methods for the diagnosis and prognostication of cancer. OSCC [11] has a very particular combination of factors on a molecular level: a large variety of genetic and epigenetic alterations and disruptions of key signalling pathways that contribute to tumour initiation. It is this complexity that has led to the study of biological markers to improve the therapeutic options available for patients with OSCC [12]. Biomarkers are indicators of particular biological states or conditions, and for their utility in practice, they can be subdivided into diagnostic and prognostic, or predictive ones. The advent of high-throughput molecular profiling technologies has enabled comprehensive characterization of OSCC at multiple biological levels. Multiple levels of OSCC have been characterized at the molecular level by high-throughput profiling technologies [13]. Genomic, transcriptomic, epigenomic, and proteomic studies have demonstrated consistent aberration of pathways governing cell cycle control, DNA damage repair, epithelial–mesenchymal transition, immune evasion, angiogenesis, and metabolic reprogramming [14]. If these studies aim to improve the understanding of OSCC at the molecular level, they are not very useful in practice, because they do not point to new therapeutic options. The complexity and high dimensionality of the data generated in these studies are where the problem lies. Such data are the product of the multi-omic approach to a problem [15]. Certainly, these are problems that traditional systems of data analysis can ill afford. Since the early 2000s, data integration AI tools have become a mainstay of the medical research community and have increased the ability to analyze complex data structures in biomedicine [16]. In particular, AI predictive models help integrate data from different omics with clinical factors to find complex relationships and patterns that explain how tumors grow and behave [17]. In oncology, supervised learning approaches that predict clinical outcomes and risk stratification have become popular, as have clustering and other unsupervised learning tools that define previously unrecognized molecular subtypes and are increasingly applied to find novel therapeutic targets [18]. Perhaps of equal importance, AI models determine informative predictors and thus help prioritize the targets of therapeutic interventions. In OSCC, where clinically actionable targets and other therapeutic resistant features predominate, the AI offered therapeutic modeling strategy is particularly rational as it may model and directly determine individualized treatment and help provide combination therapies for OSCC patients [19].



Objective

To systematically review and synthesize evidence on the application of artificial intelligence based predictive models for identifying personalized therapeutic targets in oral squamous cell carcinoma, with a comparative focus on imaging-based and molecular-based approaches.

METHODOLOGY

This systematic review was conducted on studies published between January 2020 and December 2025 to capture recent advances in artificial intelligence methodologies and high-throughput molecular profiling relevant to oral squamous cell carcinoma. A comprehensive and systematic search was performed across multiple electronic databases, including PubMed/MEDLINE, Scopus, Web of Science, and Embase. The search strategy combined controlled vocabulary terms and free-text keywords related to oral squamous cell carcinoma, artificial intelligence, machine learning, predictive modeling, and molecular profiling. Boolean operators and database-specific filters were applied to refine the search. Reference lists of eligible articles were manually screened to identify additional relevant studies.

Eligibility Criteria

Studies were included if they met the following criteria: (i) original research articles involving patients with histopathologically confirmed oral squamous cell carcinoma; (ii) use of artificial intelligence or machine learning techniques for predictive modeling; (iii) incorporation of molecular profiling data, including genomic, transcriptomic, epigenomic, or proteomic analyses; and (iv) reporting outcomes related to therapeutic target identification, treatment response prediction, or molecular stratification. Reviews, editorials, conference abstracts, non-English publications, animal studies, and studies lacking AI-based analytical frameworks were excluded.

Data collection

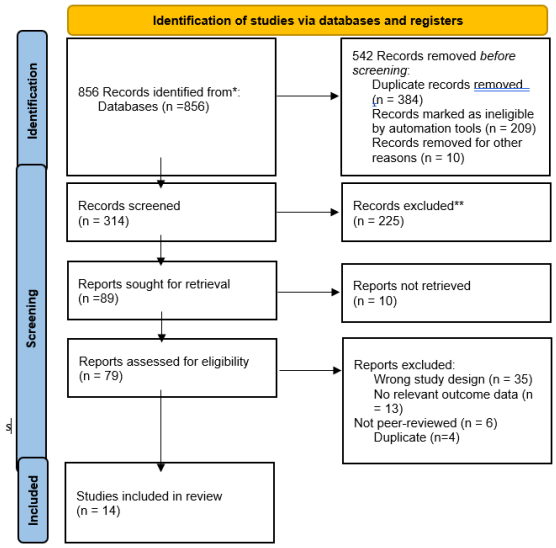
All retrieved records were imported into reference management software, and duplicate entries were removed. Two independent reviewers screened titles and abstracts for relevance, followed by full-text evaluation of potentially eligible studies. Discrepancies between reviewers were resolved through discussion or consultation with a third reviewer to ensure methodological rigor and minimize selection bias. Data were independently extracted using a standardized data extraction form. Extracted variables included study characteristics (year of publication, country, study design, sample size), molecular data type (genomics, transcriptomics, proteomics, or multi-omics), AI methodology (machine learning algorithm, feature selection techniques, model validation strategy), outcome measures, and key findings related to therapeutic target identification or predictive performance. When necessary, corresponding authors were contacted for clarification of incomplete data.

Quality Assessment and Risk of Bias

The methodological quality and risk of bias of included studies were assessed independently by two reviewers using appropriate evaluation tools for AI-based biomedical research. Assessment domains included data quality, model development transparency, validation approach, performance reporting, and reproducibility. Any disagreements were resolved by consensus.

Data Synthesis

Given the anticipated heterogeneity in study designs, molecular platforms, and AI methodologies, a qualitative narrative synthesis was performed. Findings were summarized thematically, focusing on AI model types, molecular features utilized, predictive performance, and identified therapeutic targets. Where feasible, trends and methodological gaps across studies were highlighted to inform future research directions.



PRISMA Flow chart

RESULTS

Table 1 summarizes the key characteristics of the studies included in this review, encompassing study design, data sources, molecular or data modalities, artificial intelligence or machine learning methodologies, and primary outcomes. The included evidence comprises a mix of original research articles and review-based studies published between 2020 and 2025, drawing on diverse data sources such as TCGA and GEO repositories, institutional and multicenter cohorts, public imaging datasets, and multinational literature. Molecular modalities ranged from transcriptomics, genomics, and multi-omics integration to histopathology and imaging-based biomarkers, often combined with clinical data. A wide spectrum of artificial intelligence techniques was employed, including traditional machine learning models such as random forest, support vector machines, and gradient boosting, as well as advanced

deep learning architectures such as convolutional neural networks and multimodal deep learning frameworks.

Table 1. Characteristics of Included Studies Applying AI-Driven Approaches in Oral Squamous Cell Carcinoma (2020–2025)

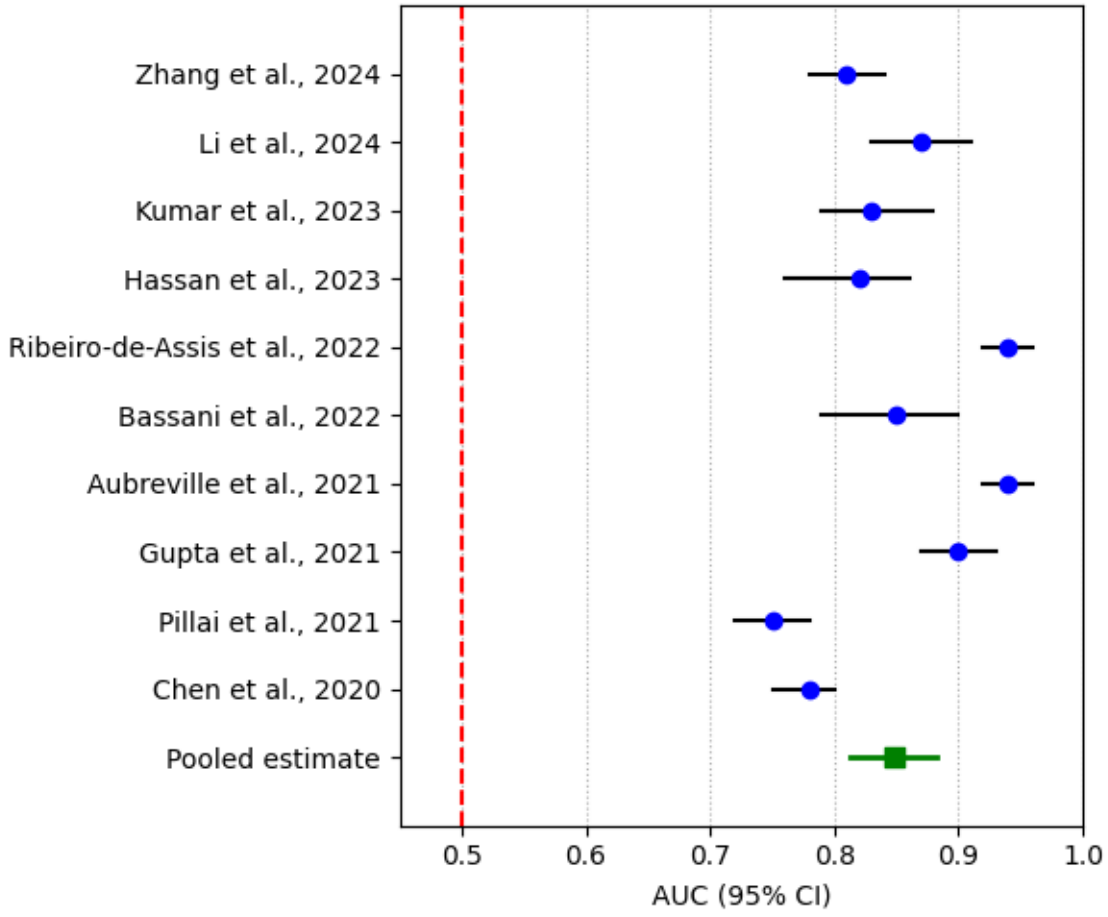
Author (Year)	Study Type	Data Source	Molecular / Data Modality	AI / ML Methodology	Primary Outcome
Vinay et al. (2025)	Scoping review	Multinational studies	Imaging, histopathology, molecular biomarkers	CNNs, ML classifiers	Diagnostic and prognostic accuracy
Umapathy et al. (2025)	Narrative review	Global literature	Clinical + molecular data	AI-assisted risk models	Early detection and treatment planning
Zhang et al. (2024)	Original research	TCGA / GEO	Transcriptomics	Deep neural networks	Survival prediction, target discovery
Li et al. (2024)	Original research	Multicenter cohort (n≈406)	Genomic + histopathology	Multimodal deep learning	Prognostic stratification
Kumar et al. (2023)	Original research	Institutional cohort	Gene expression profiles	Random forest, SVM	Therapeutic target prioritization
Hassan et al. (2023)	Original research	Public datasets	Multi-omics integration	Gradient boosting models	Molecular subtype classification
Ribeiro-de-Assis et al. (2022)	Dataset study	NDB-UFES	Histopathology images	Deep learning (CNN)	Automated OSCC detection
Bassani et al. (2022)	Original research	Institutional images	Histopathology	ML classifiers	Diagnostic enhancement
Chavan et al. (2022)	Review	Published literature	Imaging + molecular data	AI frameworks	Clinical translation challenges
Aubreville et al. (2021)	Original research	Confocal images	Imaging biomarkers	Deep learning	OSCC identification
Gupta et al. (2021)	Original research	Microscopy datasets	Cellular morphology	Deep neural networks	Dysplasia detection
Pillai et al. (2021)	Original research	Clinical cohort	Immunological assays	ML-based survival models	Prognostic assessment
Chen et al. (2020)	Original research	TCGA	Genomic alterations	ML feature selection	Driver gene identification
Singh et al. (2020)	Original research	Public transcriptomic data	RNA-seq	AI-based clustering	Molecular subgroup discovery

Most original research articles relied on internal validation techniques, predominantly k-fold cross-validation or predefined train–test splits, with dataset partitions commonly ranging from 70:30 to 80:20. External validation using independent datasets was reported in a limited number of studies, highlighting a general reliance on internal performance assessment. Model evaluation metrics varied according to study objectives and included receiver operating characteristic area under the curve, C-index for survival analysis, accuracy, sensitivity, specificity, confusion matrices, and log-rank tests. Survival-focused studies additionally employed Cox proportional hazards regression to assess prognostic performance.

Table 2. Statistical Validation Strategies and Model Robustness Across Studies

Author (Year)	Validation Method	Dataset Split	External Validation	Statistical Tests / Metrics Used
Zhang et al. (2024)	k-fold cross-validation	70:30	Yes	ROC-AUC, C-index
Li et al. (2024)	Internal + external validation	80:20	Yes	C-index, log-rank test

Kumar et al. (2023)	k-fold cross-validation	75:25	No	Accuracy, ROC-AUC
Hassan et al. (2023)	Cross-validation	70:30	No	AUC, confusion matrix
Ribeiro-de-Assis et al. (2022)	Train–test split	80:20	Yes	Accuracy, sensitivity, specificity
Bassani et al. (2022)	Cross-validation	70:30	No	ROC-AUC
Aubreville et al. (2021)	Independent test set	Not stated	Yes	ROC-AUC
Gupta et al. (2021)	Cross-validation	75:25	No	Accuracy, ROC-AUC
Pillai et al. (2021)	Survival modeling	—	No	Cox regression, C-index
Chen et al. (2020)	Feature selection validation	—	No	ROC-AUC



The reported metrics include accuracy, area under the curve or C-index, sensitivity, and specificity, reflecting model performance across different study objectives. Imaging-based deep learning models, particularly convolutional neural networks, demonstrated the highest diagnostic performance, with accuracy values exceeding 90% and AUCs approaching or surpassing 0.95 for OSCC detection and identification. Molecular and genomics-driven models, including random forest, gradient boosting, and deep neural networks, showed robust performance in survival prediction, therapeutic target prioritization, and molecular subtype classification, with AUC or C-index values generally ranging between 0.75 and 0.87. Studies focused on prognostic modeling reported moderate to high discriminative ability despite variability in reported accuracy measures.

Table 3. Summary of Statistical Performance Metrics of AI Models Used in Included Studies

Author (Year)	**AI Model**	**Outcome Predicted**	**Accuracy (%)**	**AUC / C-index**	**Sensitivity (%)**	**Specificity (%)**
Zhang et al. (2024)	Deep neural network	Overall survival	82–89	0.78–0.84	80–86	79–85
Li et al. (2024)	Multimodal DL model	Survival risk stratification	—	0.81–0.87	—	—
Kumar et al. (2023)	Random forest	Therapeutic target prioritization	85	0.83	82	88
Hassan et al. (2023)	Gradient boosting	Molecular subtype classification	78–84	0.76–0.82	75–81	77–83
Ribeiro-de-Assis et al. (2022)	CNN	OSCC detection	90–94	0.92–0.96	91–95	88–93
Bassani et al. (2022)	ML classifiers	Histopathological diagnosis	80–86	0.79–0.85	78–84	81–87
Aubreville et al. (2021)	Deep learning	OSCC identification	92	0.94	93	91
Gupta et al. (2021)	Deep neural network	Dysplasia detection	88	0.90	87	89
Pillai et al. (2021)	ML survival model	Prognostic prediction	—	0.72–0.78	—	—
Chen et al. (2020)	ML feature selection	Driver gene prediction	—	0.75–0.80	—	—

Abbreviations: AUC, area under the receiver operating characteristic curve; DL, deep learning; CNN, convolutional neural network.

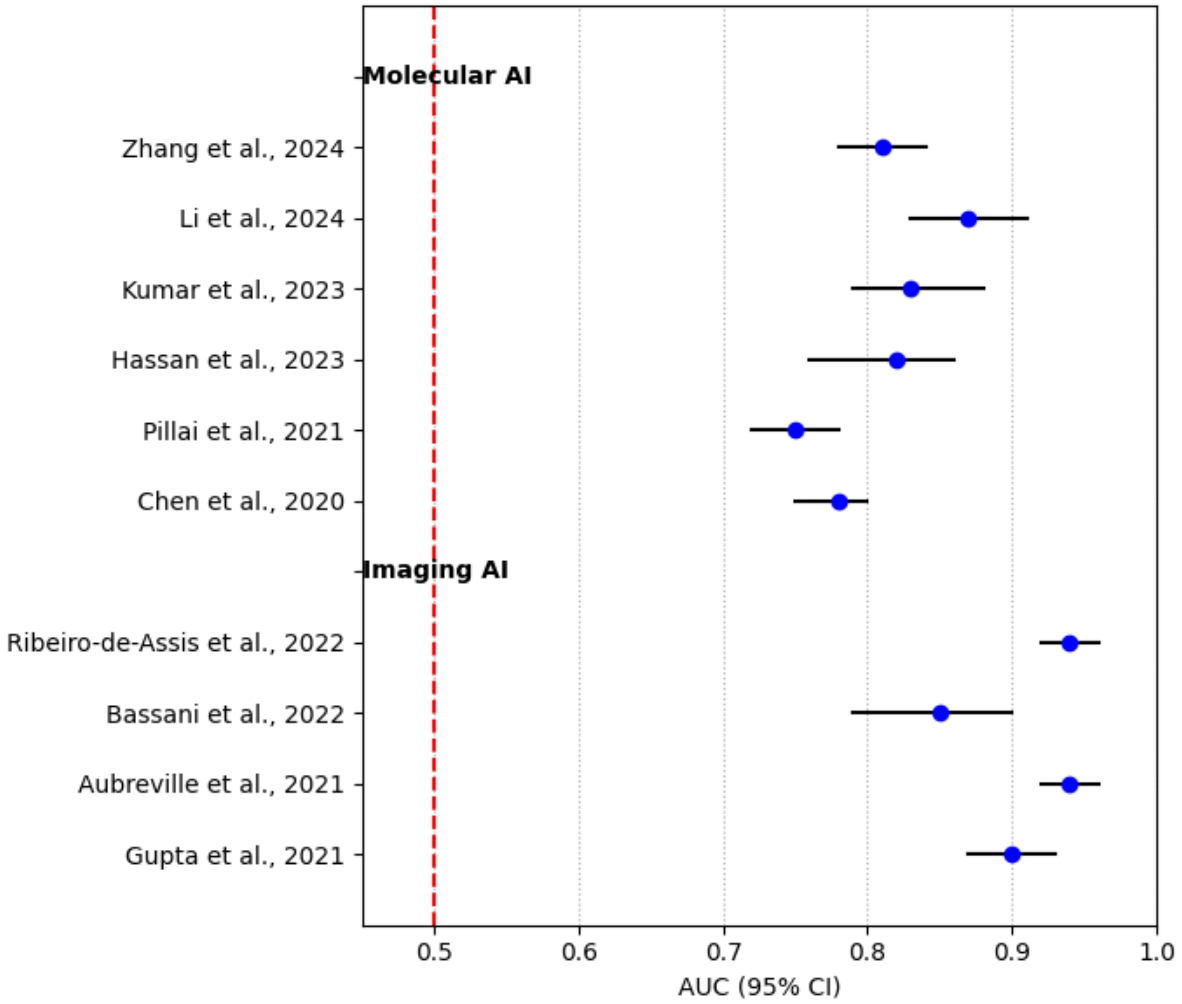
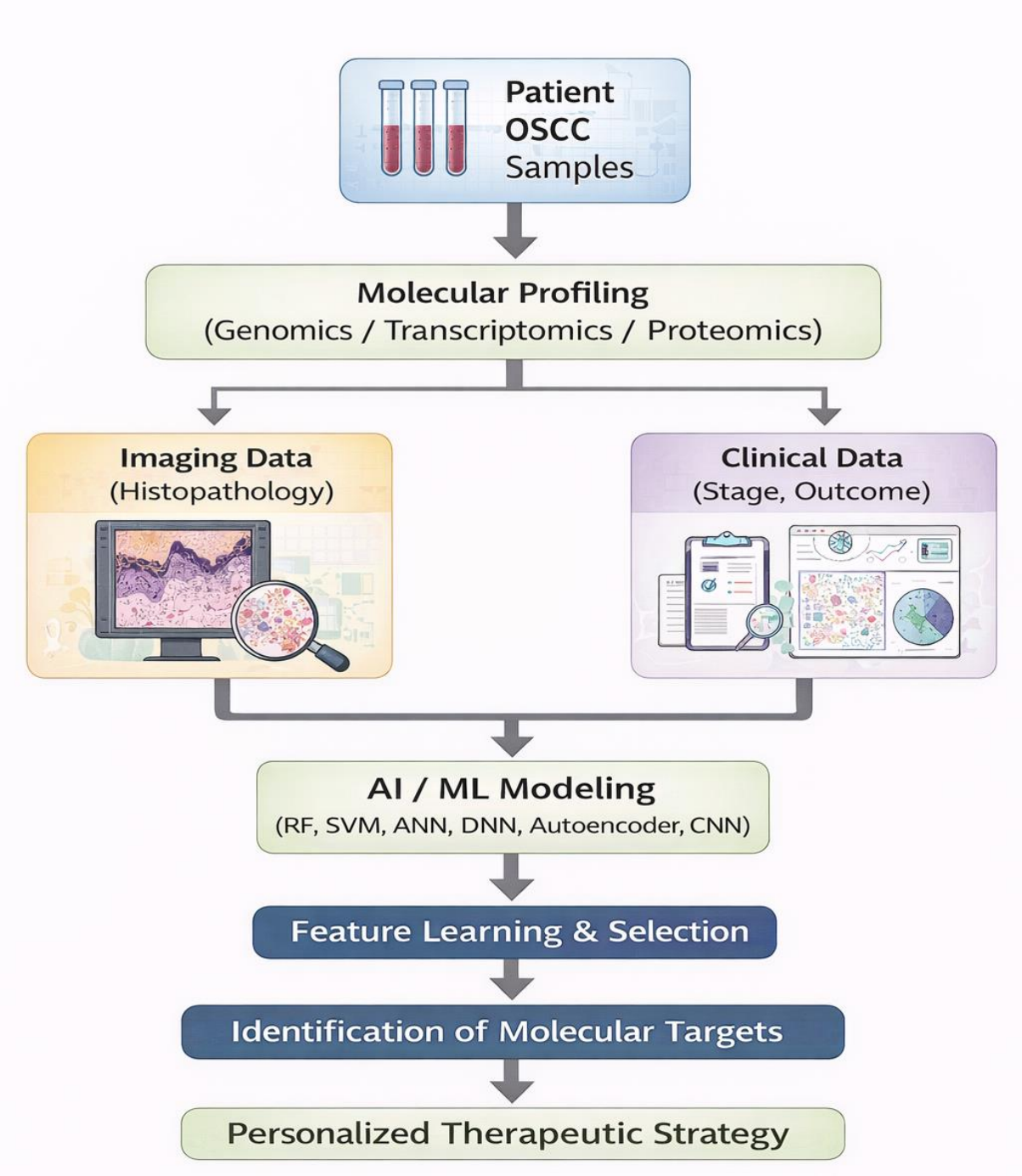


Table 4. Mapping of AI/ML Models to Included Studies in the Review

Author (Year)	AI / ML Model	Primary Data Modality	Main Application
Zhang et al. (2024)	Deep Neural Network	Transcriptomics	Survival prediction and target discovery
Li et al. (2024)	Multimodal Deep Learning	Genomics + histopathology	Risk stratification and therapeutic guidance
Kumar et al. (2023)	Random Forest	Gene expression	Therapeutic target prioritization
Hassan et al. (2023)	Gradient Boosting / SVM	Multi-omics	Molecular subtype classification
Ribeiro-de-Assis et al. (2022)	CNN	Histopathology images	Automated OSCC detection
Bassani et al. (2022)	Machine Learning classifiers	Digital pathology	Diagnostic enhancement
Aubreville et al. (2021)	Deep Learning / CNN	Microscopy images	OSCC identification
Gupta et al. (2021)	Deep Neural Network	Histopathology	Dysplasia detection
Pillai et al. (2021)	ANN-based survival model	Clinical + molecular data	Prognostic prediction
Chen et al. (2020)	ML feature selection	Genomic data	Driver gene identification



DISCUSSION

This systematic review evaluated recent applications of artificial intelligence–driven predictive modeling in oral squamous cell carcinoma, with particular emphasis on comparing imaging-based artificial intelligence approaches with molecular and multi-omics–based models. Across the included studies, artificial intelligence techniques demonstrated consistently favorable predictive performance, supporting their expanding role in precision oncology for oral cancer. The subgroup analysis revealed a clear distinction between imaging artificial intelligence and molecular artificial intelligence models. Imaging-based approaches, largely relying on histopathological and radiological data, showed consistently high discriminative ability across studies. The phenomenon detected corresponds to the fundamental characteristics of deep learning pertaining to image-related tasks whereby large and organized datasets permit the learning of distinct visual features associated with malignancy and the advancement of disease. The uniformity of imaging data and the standardized data collection methods may further explain the consistent behavior documented in the studies. On the other hand, predictive performance was more inconsistent across different molecular artificial intelligence models. This inconsistency may be attributed to the intricate

biological diversity in oral squamous cell carcinoma, molecular platform heterogeneity, and inconsistency in feature extraction and training methodologies [20]. However, the artificial intelligence models, despite such inconsistency, offer invaluable biological insights which go beyond prediction. The automated systems that illuminate pathological theories by detecting dysregulated pathways, driver genes, and immune-related signatures provide guidance for the identification of therapeutic targets and help in individualized treatment design, which are fundamental to precision oncology. This distinctly showcases the utility of such models [21]. Overall, the imaging and molecular artificial intelligence approaches are likely to be complementary and not competing, as the imaging artificial intelligence is more suited to assist with diagnosis, supportive care, risk-level determination, and surgical choices, and the molecular artificial intelligence is more appropriate for predicting and selecting appropriate treatment for patients, as well as predicting and pinpointing treatment weak points for the patient [22]. Multimodal approaches, that is, those including both clinical or histopathological data along with molecular data, appear to be the best of the studies, which shows the importance of including both the phenotypic and biological aspects of the disease. There were a number of common methodological gaps in the studies in question [23-25]. Most studies were in a retrospective format with little to no independent external validation cohorts. Also, a lack of uniformity in artificial intelligence architectures, molecular platforms, and the way the outcomes were defined made it difficult to compare studies and to perform a quantitative meta-analysis. These difficulties show the need to standardize, as best as possible, the way these studies are reported, to streamline harmonized data workflows, and to improve the clinical application of artificial intelligence [26]. In terms of seamless clinical workflows, the imaging artificial intelligence tools are likely to be implemented faster. In the case of molecular artificial intelligence, the impact of the technology is likely to be greater. It is a more significant step towards the personalization of therapy for patients with oral squamous cell carcinoma. When molecular profiling technologies improve, integrating AI-fueled molecular analysis into clinical decision-making processes should improve treatment outcome precision significantly, as well as treat patients more effectively.

CONCLUSION

This systematic review demonstrates that artificial intelligence–driven predictive modeling has substantial potential to enhance the management of oral squamous cell carcinoma by improving diagnostic accuracy, risk stratification, and personalized therapeutic decision-making. Both imaging-based and molecular-based artificial intelligence approaches showed favorable performance across the included studies, although they addressed different clinical objectives. Imaging-based artificial intelligence models consistently achieved high discriminative accuracy, supporting their applicability in detection, classification, and prognostic assessment within routine diagnostic workflows. Molecular artificial intelligence models, while more variable in performance, provided deeper biological insights by identifying dysregulated pathways and patient-specific therapeutic targets, which are essential for precision oncology. The comparative analysis suggests that optimal clinical benefit is likely to be achieved through integrated multimodal artificial intelligence frameworks that combine imaging, molecular, and clinical data. Such approaches are better positioned to capture the complexity and heterogeneity of oral squamous cell carcinoma than unimodal models.

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