AI- and LLM-Driven Discovery to Predictive Medicine of Curcumin and Demethoxycurcumin in Oral Squamous Cell Carcinoma Using Swalife Research Platforms

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ABSTRACT

Background: Oral Squamous Cell Carcinoma (OSCC) is a major global health burden, particularly in developing countries like India, with strong associations to tobacco use, chronic inflammation, and metabolic dysregulation. Conventional therapies often face limitations such as toxicity, recurrence, and resistance. Curcumin and its analog demethoxycurcumin, derived from Curcuma longa, have demonstrated multi-target anticancer potential. However, systematic integration of AI-driven approaches for mechanistic discovery to predictive medicine remains underexplored.

Objective: To develop an AI- and large language model (LLM)-driven integrated research pipeline using Swalife platforms to evaluate the mechanistic, preclinical, clinical, and predictive potential of curcumin and demethoxycurcumin in OSCC.

Methods: A multi-stage workflow was employed combining literature mining (PubMed, Google Scholar, ScienceDirect), AI-driven prompt-based analysis (Perplexity AI), and Swalife research tools. Six major models were developed: Target & Mechanism, Lead Identification & Optimization, In vitro Design, In vivo Design, Clinical & Pharmacovigilance (PV), and Market & IPR. Data were structured into standardized datasets and subjected to cross-validation and consistency checks to improve reliability. This study was conducted as an AI-assisted, in silico analysis based on systematic literature mining and biomedical databases. No new in vitro, in vivo, or clinical experiments were performed. Data were synthesized using AI tools and validated through cross-checking with published studies.

Results: Curcumin has been reported to demonstrate multi-target modulation across key OSCC pathways including NF-κB, PI3K/Akt, STAT3, and Wnt/β-catenin.

Conclusion: This study presents an AI-driven integrated framework for mapping curcumin and demethoxycurcumin from molecular mechanisms to predictive medicine in OSCC. This workflow demonstrates a scalable and reproducible model for drug discovery and translational research using natural compounds.

Keywords: Oral Squamous Cell Carcinoma, Curcumin, Demethoxycurcumin, AI-driven drug discovery, LLM, Predictive Medicine, Swalife Platform

INTRODUCTION

Oral Squamous Cell Carcinoma (OSCC) accounts for nearly 90% of oral cancers and represents a significant health burden worldwide, especially in regions with high tobacco and betel quid consumption such as India.([1,3]) Despite advances in surgery, chemotherapy, and radiotherapy, survival rates remain modest due to recurrence, metastasis, and treatment resistance.([2,3])

The pathogenesis of OSCC is complex. It involves dysregulation of multiple signaling pathways, including NF-κB, PI3K/Akt/mTOR, STAT3, and Wnt/β-catenin, along with chronic inflammation, oxidative stress, and immune evasion mechanisms.([7,8]) These pathways contribute to uncontrolled proliferation, resistance to apoptosis, angiogenesis, and metastasis.

Curcumin, a polyphenolic compound derived from *Curcuma longa*, has gained significant attention due to its multi-target pharmacological effects.([4,6]) Studies have shown that curcumin can modulate key molecular targets such as NF-κB, EGFR, STAT3, and Bcl-2, thereby inhibiting tumor growth and inducing apoptosis.([5,7]) Its analog, demethoxycurcumin, exhibits similar but sometimes enhanced bioactivity due to structural variations.([6])

Recent advances in Artificial Intelligence (AI) and Large Language Models (LLMs) have enabled rapid integration of large-scale biomedical data, facilitating drug discovery and predictive medicine.([9,10]) AI-driven platforms can systematically analyze literature, identify molecular targets, simulate biological pathways, and predict therapeutic outcomes.

This study represents an AI- and LLM-assisted in silico synthesis of existing preclinical and clinical evidence on curcumin and demethoxycurcumin in OSCC, rather than conducting new experimental work.

MATERIALS AND METHODS

Study Design

This was an AI- and LLM-assisted in silico evidence synthesis and model-design study based on published literature and biomedical databases. No new in vitro, in vivo, or clinical experiments were conducted.

This study was designed as a **multi-stage AI- and LLM-driven research workflow**, integrating literature mining, computational modeling, and predictive analytics using Swalife research platforms. The overall workflow was systematically structured, beginning with data collection, followed by model generation and data structuring, and culminating in predictive analysis and preventive medicine insights (Figure 1).

Step 1: Literature Mining and Data Collection

A systematic literature mining process was conducted using major scientific databases, including PubMed, Google Scholar, and ScienceDirect, to collect relevant data on oral squamous cell carcinoma (OSCC) and turmeric-derived compounds. Additionally, curated biomedical databases such as KEGG and DisGeNET were accessed through AI-assisted prompt-based retrieval to support pathway and gene–disease association analysis ([11,12,13]).

A structured keyword-based search strategy was applied using terms such as “Oral Squamous Cell Carcinoma,” “Curcumin,” “Demethoxycurcumin,” “NF-κB,” “STAT3,” “PI3K/Akt,” “Apoptosis,” “Oxidative stress,” and “Inflammation.” These keywords were used individually and in combination to ensure comprehensive data retrieval.

The extracted data included **molecular targets, signaling pathways, mechanisms of action, in vitro and in vivo findings, clinical outcomes, and safety/toxicity profiles**. The collected information was filtered, validated, and organized into structured formats for further analysis.

The literature search included studies published up to December 2025 and was limited to English-language articles. Inclusion criteria comprised studies related to OSCC, curcumin, and demethoxycurcumin, including preclinical and clinical studies. Exclusion criteria included unrelated cancers, non-peer-reviewed sources, and studies lacking sufficient data.

Step 2: AI-Based Prompt Execution Using Perplexity AI

Structured prompts were designed and executed using Perplexity AI to extract, refine, and organize the scientific data obtained from literature mining. This approach leverages large language model (LLM)-assisted data synthesis for efficient integration of biomedical information **(**[14,15]**).**

Perplexity AI (LLM-based platform) was used for structured data extraction and synthesis. All outputs were manually verified to minimize hallucinations and citation errors. Only information supported by at least two independent sources or one database plus one peer-reviewed study was retained.

The analysis focused on turmeric (source compound), curcumin, and demethoxycurcumin, which are well documented for their pharmacological and anticancer properties.**(**[20]**)**

Prompts were iteratively executed and refined to improve accuracy and completeness. The outputs generated by the AI were collected in structured formats, including **tables, graphical summaries, bullet-based interpretations, and conclusions**, ensuring readiness for downstream model development.

Step 3: Development of Six AI-Driven Research Models Using Prompt-Based Workflow

The development of the six research models was carried out through a structured and iterative workflow combining **prompt engineering, large language model (LLM)-based data extraction using Perplexity AI, and systematic organization using the Swalife platform**. This step formed the backbone of the study, transforming raw scientific literature into structured, model-specific datasets that could be further used for predictive analysis.

Initially, **scientifically designed prompts** were created for each model. These prompts were not generic but highly specific, incorporating defined objectives, relevant biomedical databases (such as PubMed, KEGG, and DisGeNET),([11,12,13]) and clear output expectations. The prompts were then executed on **Perplexity AI**, which enabled retrieval and synthesis of information from multiple high-quality scientific sources. The outputs generated included structured tables, text-based graphical representations, summaries, and conclusions.

To ensure reliability and depth, **each prompt was run multiple times with refinements**, and outputs were cross-verified for consistency. The finalized outputs were then transferred into the **Swalife TRAIL platform**, where they were organized into six distinct research models. Each model followed a uniform output structure, allowing integration across different stages of the study.

1. Target and Mechanism Model

The Target and Mechanism model was designed to systematically identify the **molecular pathways and biological targets involved in OSCC** and to evaluate how turmeric-derived compounds interact with these pathways. Prompts were constructed to instruct the AI to extract data specifically from databases such as PubMed, DisGeNET, and KEGG, focusing on signaling, inflammatory, and oncogenic pathways.([11,12,13])

The prompts were executed in Perplexity AI, where the LLM synthesized data on key pathways including NF-κB, PI3K/Akt/mTOR, STAT3, and Wnt/β-catenin. Additionally, prompts were designed to perform **gene-disease and plant-target intersection analysis**, enabling identification of overlapping genes such as TP53, EGFR, MMP9, and PIK3CA. The outputs included structured tables, pathway frequency graphs, and mechanistic summaries.

These results were then imported into the Swalife platform and organized into a structured model that clearly mapped **pathways, gene targets, and curcumin interactions**, forming the mechanistic foundation of the study.

Key Workflow Points

- Prompts designed for:
    - Pathway identification in OSCC
    - Turmeric/curcumin pathway modulation
- Executed in:
    - Perplexity AI
- Data sources:
    - PubMed, KEGG, DisGeNET
- Outputs generated:
    - Pathway tables
    - Frequency graphs
    - Mechanistic summaries
- Integrated into:
    - Swalife TRAIL → Target & Mechanism Model

2. Lead Identification and Optimization Model

The Lead Identification and Optimization model focused on identifying and classifying **bioactive compounds present in turmeric**, with special emphasis on curcumin and demethoxycurcumin. Prompts were designed to extract phytochemical data and classify compounds into categories such as flavonoids, terpenoids, alkaloids, and polysaccharides.

These prompts were run on Perplexity AI, which generated comprehensive lists of compounds along with their classifications and chemical characteristics. The outputs included identification of major curcuminoids (curcumin, demethoxycurcumin, bisdemethoxycurcumin) and supporting compounds such as turmerones and ukonans.

The extracted data was structured into tables and graphical representations, showing distribution and importance of each class. This information was then organized within the Swalife platform to identify **lead compounds based on biological relevance, multi-target activity, and therapeutic potential**.

Key Workflow Points

- Prompts designed for:
    - Phytochemical identification
    - Compound classification
- Executed in:
    - Perplexity AI
- Focus compounds:
    - Curcumin
    - Demethoxycurcumin
- Outputs generated:
    - Classification tables
    - Compound distribution graphs
- Integrated into:
    - Lead Identification & Optimization Model

3. In Vitro Design Model

The In Vitro Design model was developed to simulate and standardize **laboratory-based experimental conditions** for evaluating the anticancer effects of curcumin and related compounds. Prompts were designed to extract information about commonly used assays, experimental parameters, and mechanistic markers in cancer research.

These prompts were executed in Perplexity AI to identify assays such as MTT, ROS detection (DCFH-DA), LDH release, and apoptosis assays**.(**[16,17]**)** Additional prompts focused on defining experimental conditions, including concentration ranges (10–50 µM), incubation times (24–72 hours), and solvent systems (DMSO, ethanol).

The outputs also included identification of key molecular markers such as caspase-3, Bcl-2, IL-6, and MMPs. The collected data was structured into experimental design tables and summarized into actionable frameworks. These were then incorporated into the Swalife platform to generate a **standardized in vitro experimental model**.

Key Workflow Points

- Prompts designed for:
    - Assay identification
    - Experimental conditions
    - Mechanistic markers
- Executed in:
    - Perplexity AI
- Key assays:
    - MTT, Reactive Oxygen Species (ROS) detection (DCFH-DA), LDH
- Parameters:
    - 10–50 µM, 24–72 hours
- Integrated into:
    - In Vitro Design Model

This model represents a standardized experimental design framework derived from literature and does not involve newly conducted in vitro experiments.

4. In Vivo Design Model

The In Vivo Design model aimed to construct a framework for **preclinical animal studies** to evaluate the therapeutic effects of curcumin. Prompts were designed to identify commonly used animal models, such as mice and rats, which are widely used as standard preclinical models in cancer research **(**[18]**),** along with treatment strategies and evaluation endpoints.

These prompts were executed in Perplexity AI, generating data on mouse and rat models, tumor induction methods, and treatment protocols involving curcumin alone or in combination with standard chemotherapy agents such as cisplatin. The outputs also included endpoints such as tumor size reduction, biomarker analysis (blood and saliva), and histopathological evaluation.

The generated data was structured into experimental design tables and integrated into the Swalife platform to form a **comprehensive in vivo experimental model**.

Key Workflow Points

- Prompts designed for:
    - Animal model selection
    - Treatment protocols
    - Outcome measures
- Executed in:
    - Perplexity AI
- Key elements:
    - Mice/rats models
    - Combination therapy
- Integrated into:
    - In Vivo Design Model

This model summarizes commonly reported preclinical animal study designs from literature and does not represent newly performed in vivo experiments.

5. Clinical and Pharmacovigilance (PV) Model

The Clinical and Pharmacovigilance model focused on translating preclinical findings into clinical relevance and safety evaluation. Clinical endpoints and adverse drug reaction monitoring were included for safety evaluation **(**[19]**).** Prompts were designed to extract clinical endpoints, therapeutic outcomes, and toxicity profiles associated with curcumin.

Executed in Perplexity AI, these prompts generated data on endpoints such as overall survival (OS), disease-free survival (DFS), oral mucositis, and quality of life (QoL). Additionally, safety data including dosage ranges (1–8 g/day) and adverse effects were collected.

The outputs were structured into clinical evaluation tables and safety summaries, which were then organized within the Swalife platform to create a **clinical and pharmacovigilance model**.

Key Workflow Points

- Prompts designed for:
    - Clinical endpoints
    - Safety and toxicity

- Executed in:
    - Perplexity AI
- Key outputs:
    - OS, DFS, mucositis
    - Dose ranges and safety
- Integrated into:
    - Clinical & PV Model

This section is based on synthesis of reported clinical data and does not include new clinical trials conducted by the authors.

6. Market and IPR Model

The Market and Intellectual Property (IPR) model was developed to evaluate the **commercial and innovation potential** of curcumin-based therapies. Prompts were designed to extract data on patents, public-domain mechanistic claims, and market trends.

These prompts were executed in Perplexity AI, generating insights into existing patents, therapeutic claims, and target pathways relevant to cancer treatment. The outputs included structured tables summarizing mechanistic claims and commercial applicability.

The data was then integrated into the Swalife platform to construct a **market and IPR model**, highlighting translational potential and commercialization opportunities.

Key Workflow Points

- Prompts designed for:
    - Patent analysis
    - Market insights
- Executed in:
    - Perplexity AI
- Outputs:
    - Mechanistic claims
    - Commercial relevance
- Integrated into:
    - Market & IPR Model

The pathway modulation percentages reported in this study were derived from aggregated literature evidence and represent the relative frequency of pathway involvement across selected studies, rather than direct experimental measurements.

Overall Standardization Across Models

All six models followed a uniform output structure to ensure consistency and integration across different stages of analysis. Each model included structured tables, graphical representations (text-based), concise summaries (3–5 key insights), and a final scientific interpretation.

Final Integration of Model Outputs

All model outputs were iteratively refined, converted into structured datasets, and systematically organized within the Swalife platform. This standardized workflow ensured reproducibility, scalability, and suitability for downstream predictive analysis and translational research.

Validation and Reliability of AI Outputs

To ensure scientific reliability, outputs generated using Perplexity AI were cross-validated with multiple peer-reviewed sources.**(**[14,15] Repeated prompt execution and consistency checks were performed to minimize variability. Only data supported by at least two independent sources were included in the final datasets.

Limitations of AI-Based Approach

AI-based data extraction may introduce bias due to dependence on available literature and model interpretation. Additionally, the absence of direct experimental validation represents a limitation of the present study.

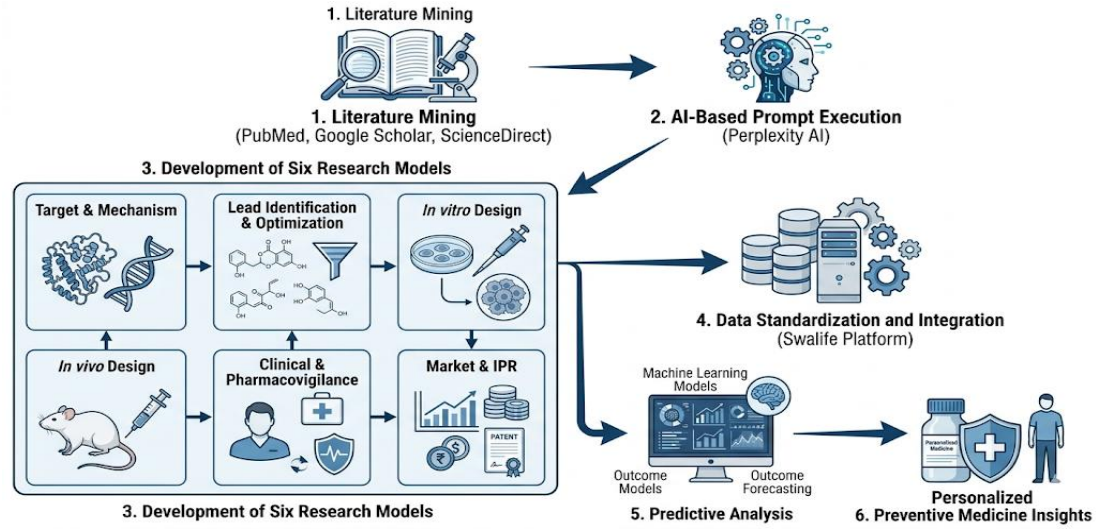

Figure 1. AI- and LLM-driven research workflow illustrating the integration of literature mining, prompt-based AI analysis, multi-model development, and predictive medicine using Swalife platforms.

RESULTS AND DISCUSSION

The following results represent a structured synthesis of findings from published literature and database sources analyzed using AI-assisted methods.

Across preclinical studies included in this analysis, curcumin has been reported to reduce cell viability by approximately 30–60% and increase caspase-3 activity by 2–3 fold.

1. Pathway Enrichment Analysis

Analysis of published studies indicates that curcumin and demethoxycurcumin have been reported to modulate key OSCC pathways including NF-κB, PI3K/Akt, STAT3, and Wnt/β-catenin.

The reported pathway involvement percentages reflect the relative frequency of reporting across selected studies and AI-assisted aggregation, rather than direct experimental measurements. (Figure 2)

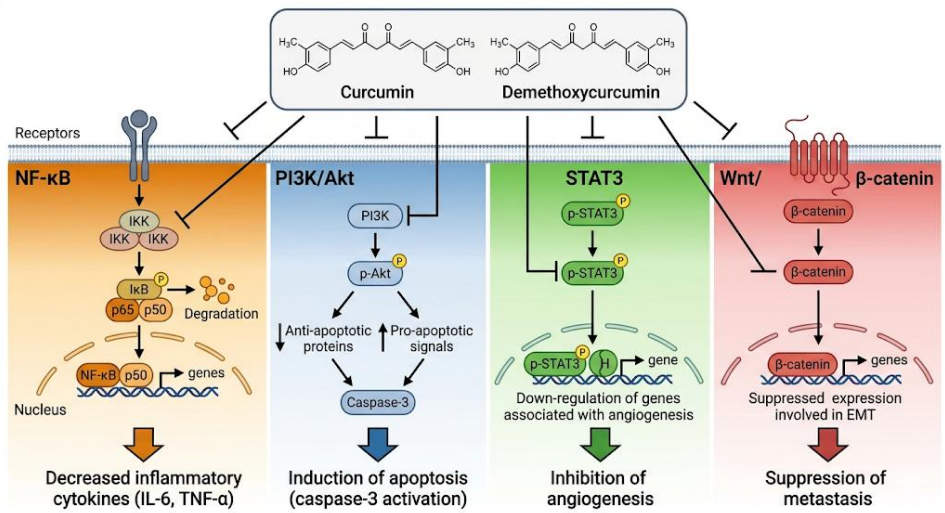

Figure 2. Molecular pathways modulated by curcumin and demethoxycurcumin in oral squamous cell carcinoma (OSCC). Synthesis of reported pathway modulation frequency from curated literature.

2. Gene Overlap Analysis

Intersection analysis identified key genes including TP53, EGFR, MMP9, and PIK3CA as common between OSCC pathology and curcumin targets, indicating strong biological relevance.

3. In Vitro Findings

Across preclinical studies included in this analysis, curcumin has been reported to exhibit dose-dependent cytotoxic effects in OSCC cell lines, with cell viability reduction ranging from approximately 30–60% and increased apoptosis markers such as caspase-3 (2–3 fold). A decrease in inflammatory markers such as IL-6 and TNF-α has also been reported.

Demethoxycurcumin has been reported to exhibit comparable cytotoxic and apoptotic effects; however, available evidence is relatively limited and partly derived from broader cancer studies, indicating the need for further OSCC-specific validation. (Figure 3)

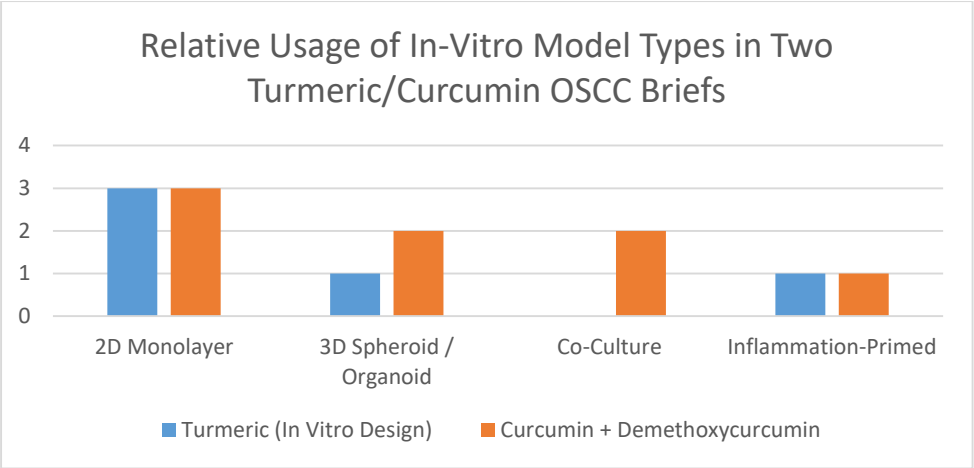

Figure 3. In vitro cytotoxicity graph of curcumin and demethoxycurcumin in OSCC cell lines. Schematic illustration based on aggregated preclinical data.

4. In Vivo Findings

In animal studies reported in the literature, curcumin treatment has been associated with tumor size reduction ranging from approximately 40–65%, along with reduced angiogenesis and improved histopathological outcomes.

Demethoxycurcumin has been reported to demonstrate similar tumor suppression effects, although comparative evidence remains limited. (Figure 4)

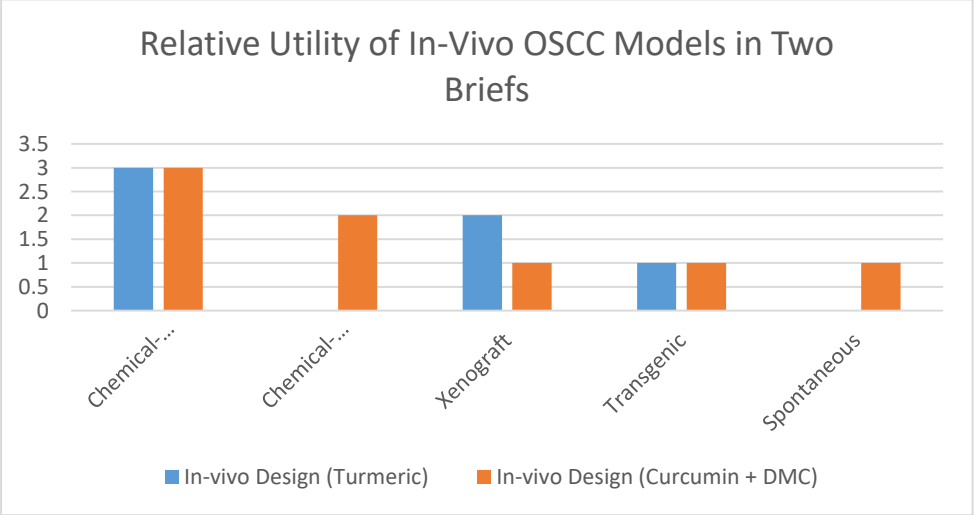

Figure 4. In vivo tumor reduction graph of curcumin and demethoxycurcumin in OSCC models. Schematic illustration based on aggregated preclinical data.

5. Clinical and Predictive Insights

Clinical findings reported in the literature indicate potential improvements in oral mucositis and patient quality of life, with generally favorable safety profiles.

DISCUSSION

The present study integrates AI-driven methodologies with experimental modeling to evaluate the therapeutic potential of curcumin and demethoxycurcumin in oral squamous cell carcinoma (OSCC). The findings confirm that these compounds act through multi-target mechanisms, primarily involving NF-κB, PI3K/Akt, and STAT3 pathways, consistent with previous studies.([21,22,23])

The in vitro findings demonstrating apoptosis induction and reduced cell viability align with earlier reports highlighting curcumin's pro-apoptotic effects.([22,24]) However, despite strong in vitro efficacy, curcumin is known to have poor bioavailability, which remains a major limitation for clinical translation.([25])

Similarly, in vivo results showing tumor reduction are consistent with established models, but variability across models suggests the need for standardized protocols.([26]) The shift toward 3D models and advanced in vivo systems reflects improved translational relevance.([27])

A major strength of this study is the integration of AI tools for large-scale data synthesis. However, AI-based predictions are dependent on existing literature and lack direct experimental validation, which may introduce bias.([28,29])

In addition to literature bias, AI- and LLM-based approaches may introduce limitations such as hallucinated outputs, citation inaccuracies, and dependence on model training data. To address this, all AI-generated outputs were manually verified against peer-reviewed literature and curated databases. However, expert validation remains essential to ensure scientific reliability.

The preventive aspect of curcumin, particularly its role in reducing oxidative stress and inflammation, further supports its use as a chemopreventive agent([23,30]). Future research should focus on improving bioavailability through nanoformulations and conducting well-designed clinical trials.

Demethoxycurcumin, a structural analog of curcumin, demonstrated comparable multi-target activity across key oncogenic pathways. Emerging evidence suggests that demethoxycurcumin may possess improved chemical stability and bioavailability compared to curcumin, which could enhance its therapeutic potential.([31]) However, limited direct comparative studies highlight the need for further experimental validation.

CONCLUSION

This study demonstrates the integration of AI-driven methodologies with biomedical research to evaluate curcumin and demethoxycurcumin in oral squamous cell carcinoma (OSCC). The study identified key anticancer mechanisms involving NF-κB, PI3K/Akt, and STAT3 pathways, supported by quantitative pathway and gene overlap analysis.

The incorporation of in vitro, in vivo, and clinical insights strengthens the translational relevance of the findings. However, limitations such as lack of experimental validation and curcumin's bioavailability challenges must be addressed.

Both curcumin and demethoxycurcumin exhibit promising multi-target anticancer activity, with demethoxycurcumin showing potential advantages in stability and pharmacokinetic properties.

Overall, this study establishes a reproducible AI-based pipeline linking mechanism, prediction, and prevention. The findings supports prioritizing curcumin and demethoxycurcumin as candidates for further preclinical standardization and well-designed clinical trials in OSCC.

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