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GC-MS phytochemical profiling and molecular docking of *Merremia tridentata* against glucosyltransferases for oral healthcare applications

Ayeesha Lubaba M, Nivedha V, Deepak Muthu S, Sathiya Balan G*
Department of Pharmacognosy, College of Pharmacy, Madurai Medical College, Madurai, Tamilnadu, India

Abstract
The present study investigated the phytochemical profile of the ethanolic extract of *Merremia tridentata* (EEMT) using Gas Chromatography-Mass Spectrometry (GC-MS) and evaluated its antimicrobial and anti-plaque potential against *Streptococcus mutans* through molecular docking. GC-MS analysis revealed the presence of several bioactive compounds including alkaloids, flavonoids, terpenoids, and phenolic derivatives. Key constituents identified were Quercetin 3,7-diglucoside, 2,4-Di-tert-butylphenol, Pyrrolidine-2,4-dione, and Phytol, which were selected for in silico analysis. Molecular docking was carried out against *S. mutans* glucosyltransferases GtfB, enzymes essential for biofilm formation and cariogenicity. The docking results showed strong binding affinities, with [insert best compound] exhibiting the highest interaction score and stable hydrogen bonding within the active sites. These findings correlate well with the *in vitro* antimicrobial activity of EEMT and suggest its potential as a natural therapeutic agent for preventing dental caries by targeting key virulence enzymes of *S. mutans*.

Keywords: Merremia tridentate, ethanolic extract, GC-MS analysis, phytochemical profile, bioactive compounds, molecular docking, *Streptococcus mutans*

Introduction

Dental caries is a chronic, biofilm-mediated infectious disease that remains a major global oral health concern. A key contributor to its pathogenesis is *Streptococcus mutans*, a Gram-positive facultative anaerobic bacterium predominantly involved in the formation of dental plaque. This bacterium adheres to the tooth surface and synthesizes extracellular polysaccharides from dietary sucrose using glucosyltransferase enzymes. These enzymes particularly GtfB and GtfC play a critical role in bacterial adhesion and biofilm maturation, making them promising molecular targets for anti-caries interventions [1].

The increasing concern over antimicrobial resistance and the side effects associated with conventional oral care agents has led to a growing interest in safer, plant-based alternatives. Medicinal plants, rich in bioactive secondary metabolites, offer a vast source of antimicrobial compounds capable of inhibiting key virulence mechanisms of pathogenic bacteria. Among these, *Merremia tridentata* (Family: Convolvulaceae) is a traditionally used medicinal herb known for its antioxidant, anti-inflammatory, and antimicrobial activities. Despite its established ethnomedicinal uses, its potential role in oral health particularly in plaque inhibition remains largely unexplored [2].

In recent years, analytical techniques such as Gas Chromatography–Mass Spectrometry (GC-MS) have enabled the rapid identification of phytoconstituents present in medicinal plant extracts. This technique allows the profiling of volatile and semi-volatile compounds that contribute to the therapeutic properties of plants [3]. Complementing this, molecular docking serves as a powerful in silico approach to predict the interaction between plant-derived compounds and specific microbial targets. Such integrative studies not only validate traditional claims but also help identify potential lead compounds for drug development.

Molecular docking is a computational method used to predict the binding interactions between small molecules (ligands) and target proteins, offering critical insights into their potential biological activities [4]. This study utilized molecular docking to assess how the main phytoconstituents of the ethanolic extract of *Merremia tridentata* (EEMT) interact with key virulence enzymes of Streptococcus mutans. The primary target enzyme relevant to anti-plaque activity is glucosyltransferases (Gtf), which catalyzes the synthesis of glucans from dietary sucrose, playing a critical role in plaque formation and bacterial adherence [5, 6].

Table 1: Comparative Overview of Glucosyltransferases (GtfS, GtfB, GtfC, GtfD)

Enzyme	Full Name	Primary Function	Glucan Type Produced	Role in Biofilm Formation	Mechanism Summary
GtfB	Glucosyltransferase B	Synthesizes water-insoluble glucans (WIG)	Mainly α-1,3-glucans	Strongly involved in adhesion to tooth surfaces and matrix	Transfers glucose from sucrose to form α-1,3 linkages; initiates biofilm matrix
GtfC	Glucosyltransferase C	Produces both soluble and insoluble glucans	α-1,3 and α-1,6-glucans	Helps in both initial attachment and biofilm maturation	Has dual activity; forms a mix of glucans aiding structural complexity
GtfD	Glucosyltransferase D	Synthesizes water-soluble glucans (WSG)	Mainly α-1,6-glucans	Assists in the early stages of biofilm formation and EPS spread	Adds glucose units via α-1,6 linkage to generate soluble glucans
GtfS	Glucosyltransferase S (less studied, species-specific)	May be involved in alternative glucan synthesis in some strains	Likely soluble or mixed glucans	Role less defined; may support extracellular polysaccharide (EPS) production	Presumed to act like GtfD but in different environmental or strain-specific conditions

Among them, GtfB was selected as primary target due to their central roles in plaque development. Thus, targeting GtfB with phytocompounds from *Merremia tridentata* may disrupt biofilm formation and reduce the cariogenic potential of *S. mutans*, making them key molecular targets in this anti-plaque investigation.

This study aims to investigate the phytochemical constituents of the ethanolic leaf extract of *Merremia tridentata* (EEMT) through GC-MS analysis and evaluate its anti-plaque activity against *Streptococcus mutans* using molecular docking. The focus is particularly on inhibiting the activity of glucosyltransferase enzyme GtfB. The combined application of phytochemical screening and computational docking aims to provide scientific insights into the oral health potential of *Merremia tridentata* and support its use as a natural therapeutic agent in dental care.

Material and Method

Collection of plant

Fresh leaves of *Merremia tridentata* (Family: Convolvulaceae) were collected during the early monsoon season (June 2025) from two locations in Tamil Nadu, India U. Vadipatti in Madurai district (Latitude: 10.2346° N, Longitude: 78.1231° E, Altitude: ~202 m) and Mettupatti in Pudukottai district (Latitude: 10.3802° N, Longitude: 78.8006° E, Altitude: ~187 m). The regions have a tropical climate, with average temperatures ranging from 28°C to 34°C during the collection period.

Authentication

The *Merremia Tridentata* plant sample was authenticated by Dr. D. Stephen, Department of Botany, The American College, Madurai.

Solvent extraction

Fresh, healthy leaves of *Merremia tridentata* were collected, washed thoroughly with distilled water, shade-dried, and ground into a coarse powder. The powdered leaves were initially defatted with petroleum ether for a period of 48 to 72 hours. After defatting, the residue was subjected to maceration using ethanol as the solvent, owing to its high polarity and efficiency in extracting a broad range of phytochemicals. About 100 g of the defatted powder was soaked in 400 ml of ethanol in a conical flask, sealed, and kept on a rotary shaker at room temperature for 48–72 hours. Following extraction, the mixture was filtered using Whatman No.1 filter paper, and the filtrate was concentrated under reduced pressure using a rotary evaporator to obtain the crude ethanolic extract of *Merremia tridentata* (EEMT). The extract was stored at 4 °C until subsequent phytochemical and biological analyses could be performed [7].

GCMS Analysis

The ethanolic extract of *Merremia tridentata* (EEMT) was analyzed using Gas Chromatography–Mass Spectrometry (GC-MS) to identify the bioactive compounds. The analysis was performed on a GC-2010 system under the following conditions [8]

Instrument and Injection Parameters

- **Injection mode:** Split
- **Injection temperature:** 250 °C
- **Split ratio:** 10.0
- **Dwell time:** 0.3 seconds
- **Washing volume:** 6 µL

Column and Carrier Gas Flow

- **Flow control mode:** Linear velocity
- **Carrier gas pressure:** 68.1 kPa
- **Column flow rate:** 1.20 ml/min

Oven Temperature Program

- **Initial temperature:** 50 °C
- **Ramp rate:** 6.0 °C/min
- **Final temperature:** 280 °C

Detector and Interface Settings

- **Ion source temperature:** 200 °C
- **Interface temperature:** 250 °C
- **Solvent cut time:** 3.5 minutes

Compound Identification

- The resulting mass spectra were analyzed using the NIST library database to identify phytochemical constituents based on similarity index and retention time.

Molecular docking analysis

The bioactive compounds identified from the GC-MS analysis of *Merremia tridentata* ethanolic leaf extract (EEMT) were selected for molecular docking studies to assess their binding affinity with key virulence-associated target proteins of *Streptococcus mutans*. The 3D structures of the compounds were retrieved from the PubChem database in SDF format and converted to PDB format using Open Babel. The crystal structure of the target protein, glucosyltransferase (GtfB), was obtained from the Protein Data Bank (PDB). Prior to docking, both ligands and proteins were prepared by removing water molecules, adding hydrogen atoms, and assigning charges using Docking studio Tools. Docking was carried out using Pyrx Vina to predict the binding affinity (in kcal/mol) and possible binding interactions. Docking poses with the lowest binding energies were selected and visualized using Discovery Studio Visualizer to analyze their binding orientations and interaction sites [9].

Result and Discussion

GC-MS Analysis

The ethanolic extract of *Merremia tridentata* (EEMT) was subjected to GC-MS analysis to determine its phytochemical constituents. The chromatogram revealed the presence of 32 distinct bioactive compounds with varying retention times and area percentages. The major constituents included propane, 2,2-diethoxy- (44.49%), 1,2,4-butanetriol (5.28%), quercetin-3-(2G-rhamnosylrutinoside) (5.2%), and methyl salicylate (2.54%). Notably, several compounds with known antimicrobial and anti-inflammatory properties were identified, such as quercetin, Kaempferol, phytol, pyrrolidine-2,4-dione, and 2,4-di-tert-butylphenol.

These secondary metabolites belong to diverse chemical classes including flavonoids, terpenoids, alkaloids, and phenolic derivatives, many of which have been associated with antibacterial and anti-plaque activities. The presence of these compounds underscores the therapeutic potential of *Merremia tridentata* in dental applications.

Table 2: GCMS Analysis of *Merremia Tridentata*

S. No	R. Time	Area	Area %	Molecular Formula	Molecular Weight (g/mol)	Compound Name
1	15.661	150349	0.27	$C_{14}H_{22}O$	206.32	2,4-Ditertbutyl phenol
2	10.6	1200000	5.2	C39H50O25	918.8	Quercetin-3-(2G- rhamnosylrutinoside)
3	12.1	850000	3.7	C36H36017	740.7	Kaempferol-3- O-(6-p- coumaroyl)-glycoside
4	22.109	177524	0.32	$C_{20}H_{40}O$	296.5	Phytol
5	6.319	1515863	2.71	$C_4H_5O_2$	99.09	Pyrrolidine-2,4-dione
6	20.681	534901	0.96	$C_{16}H_{32}O_2$	256.42	Hexadecanoic acid
7	31.25	2,450,000	20.4	C18H32O	264	9,12,15-Octadecatrienoic acid
8	8.851	37142320	2.54	$C_8H_8O_3$	152.15	Methyl salicylate
9	8.422	148432	0.27	$C_7H_{12}N_2O_2$	156.19	1-(2-Ethyl crotonyl) urea
10	7.171	199291	0.36	$C_7H_{14}O_4$	162.18	3-ethoxy, 2-Propenoic acid ethyl ester
11	12.645 1	1484045	2.16	C13H17NO3	235	Phenmetrazine carbamate
12	12.757	986145	1.43	C8 H16O6	208.21	alpha. -Methyl 4-O-methyl-D-mannoside
13	7.115	215801	0.39	$C_9H_{20}O_2$	160.25	Pentane, 1,1-diethoxy-
14	3.599	24865963	44.49	$C_7H_{16}O_2$	132.2	Propane, 2,2-diethoxy-
15	8.479	187406	0.34	$C_{10}H_{22}O_{22}$	174.28	Butane, 1,1-diethoxy-3-methyl-
16	9.307	720033	1.29	$C_9H_{20}O_3$	176.25	Propane, 1,1,3-triethoxy-
17	12.920	2948894	5.28	$C_{14}H_{10}O_3$	106.12	1,2,4-Butanetriol
18	3.266	324422	0.58	$C_5H_{12}O$	88.15	1-Butanol, 3-methyl-
19	5.083	2309236	4.13	$C_6H_{12}O_2$	116.16	2-Butenoic acid, ethyl ester, (Z)-
20	4.804	616479	1.10	$C_7H_{16}O$	116.20	3-HEXANOL, 3-METHYL-
21	20.070	192445	0.34	$C_{14}H_{22}N_2O$	234.34	Lidocaine
22	12.565	947606	1.38	C9H19N	141	N-(2-Methylbutylidene) isobutylamine
23	12.720	1701703	2.48	C8H16O6	208	2-Trimethylsiloxy-6-hexadecenoic acid, methyl ester
24	12.805	1568847	2.28	C13H11N3O3	257	2,3-Quinoxalinedione, 1,4-dihydro-1-(3 isoxazolylmethyl)-
25	12.895	3385265	4.92	C9H16O4S2	252	Methylenebis (ethyl thioglycolate)
26	12.920	2393114	3.48	C4H10O3	106	1,2,4-Butanetriol
27	13.030	287676	0.42	C5H11NO3	133	Norvaline, 3-hydroxy-
28	13.070	128543	0.19	C9H18O3	174	1,3-Pentanediol, 2-methyl-, 1-propanoate
29	16.666	174029	0.25	C14H14O4	246	Phthalofyne
30	19.391	108810	0.16	C10H18	138	Bicyclo [3.1.1] heptane, 2,6,6-trimethyl-
31	27.269	181437	0.26	C15H22N2O2	262	4-[4-morpholinyl(phenyl)methyl] morpholine

GC-MS analysis of the ethanolic extract of *Merremia tridentata* (EEMT) revealed 31 bioactive compounds, including major ones like propane, 2,2-diethoxy- (44.49%), 1,2,4-butanetriol, quercetin derivatives, 2,4-di-tert-butylphenol, and methyl salicylate. These belong to chemical classes such as flavonoids, phenolics, terpenoids, and alcohols.

The GC-MS analysis of *Merremia tridentata (L.) Hallier f.,* a medicinal plant traditionally used in the treatment of inflammation, wounds, and fever, revealed the presence of various bioactive phytoconstituents with potential pharmacological properties. The volatile profile showed the presence of multiple secondary metabolites, including alkaloids, flavonoids, fatty acids, terpenoids, esters, and phenolic compounds.

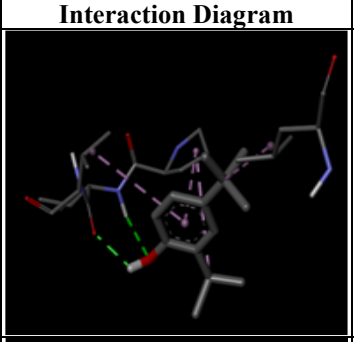
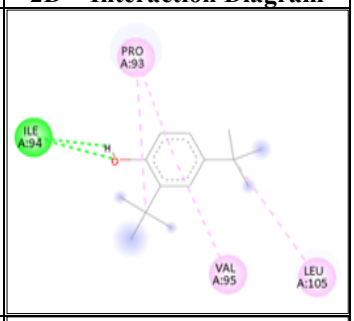
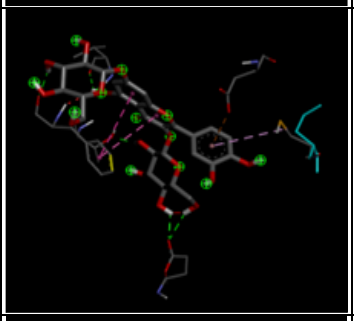
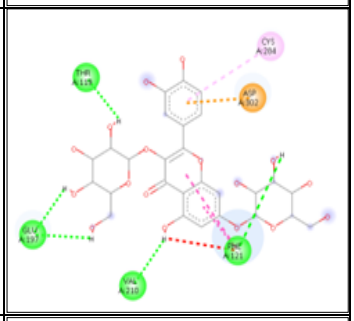
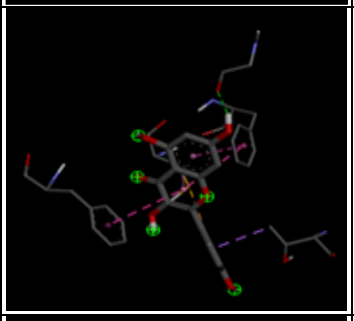
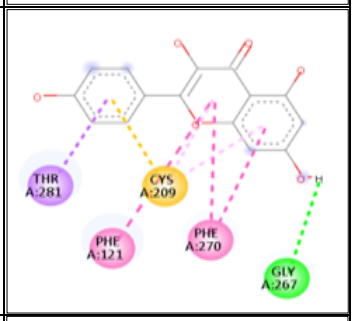
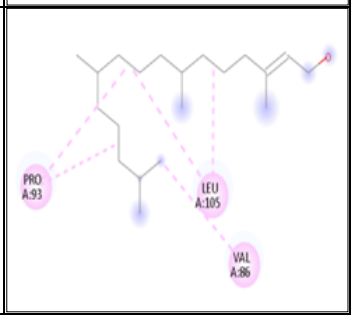
Several identified compounds are known for their antimicrobial and anti-biofilm activities, especially against *Streptococcus mutans*, the main bacterium involved in dental plaque. For example, quercetin and Kaempferol possess strong antibacterial and antioxidant properties, supporting the anti-plaque potential of the extract.

The plant's phytochemical diversity suggests it could serve as a source for developing herbal formulations and natural drugs. The GC-MS analysis thus provides scientific backing to its therapeutic potential and paves the way for further studies involving bioactivity-guided isolation, toxicological profiling and clinical validation.

These findings support the traditional medicinal applications of *Merremia tridentata* and highlight its potential as a natural agent for oral healthcare. These findings also provide a foundation for further biological and molecular docking studies.

Molecular Docking Analysis

Molecular docking was conducted to assess the interaction between key phytocompounds and glucosyltransferase enzymes (GtfB) of *Streptococcus mutans*, which are responsible for synthesizing extracellular glucans critical to plaque formation.

S. No	Phytoconstituents	Binding energy (Kcal/mol)	Interaction Diagram	2D – Interaction Diagram
1	2,4-ditert butyl phenol	-8.3		
2	Quercetin	-5		
3	Kaempferol	-6		
4	Phytol	-7.1		

Molecular docking revealed that phytocompounds from *Merremia tridentata*, such as quercetin derivatives, 2,4-di-tert-butylphenol, showed good binding affinity with GtfB enzymes of *Streptococcus mutans*. These enzymes are critical for glucan synthesis and biofilm formation. The results suggest that these compounds can potentially inhibit plaque formation by disrupting bacterial adhesion and biofilm maturation, supporting the anti-plaque potential of the extract. These findings support the traditional use of *Merremiatridentata* in oral health and warrant further biological validation through *in vitro* and *in vivo* studies.

Conclusion

This study provides scientific validation for the traditional use of *Merremia tridentata* in oral healthcare, particularly against dental plaque and caries caused by *Streptococcus mutans*. The ethanolic leaf extract (EEMT) was subjected to Gas Chromatography-Mass Spectrometry (GC-MS) analysis, which revealed the presence of various phytochemicals, including flavonoids, alkaloids, terpenoids, and phenolic compounds. Notable constituents such as quercetin, Kaempferol, phytol, and 2,4-di-tert-butylphenol are known for their antimicrobial and anti-inflammatory properties, which contribute to the plant's therapeutic potential.

To understand the molecular basis of the extract's anti-plaque activity, molecular docking studies were carried out targeting key virulence enzymes—glucosyltransferases GtfB produced by *S. mutans*. These enzymes are critical for synthesizing glucans that facilitate bacterial adhesion and biofilm maturation. Docking simulations showed that major compounds from the extract exhibited strong binding affinities to the active sites of GtfB, suggesting their potential to inhibit plaque formation at the molecular level.

The integration of phytochemical profiling with in silico docking supports the hypothesis that *M. tridentata* contains bioactive molecules capable of disrupting key mechanisms in dental plaque development. This dual approach not only enhances our understanding of the plant's pharmacological actions but also identifies lead compounds for future formulation of plant-based dental therapeutics. However, further *in vitro* and *in vivo* validations are warranted to explore its therapeutic applicability as a safe, plant-based alternative in dental care formulations.

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