The antibacterial activity of Barangan (*Musa acuminata* Colla) peel on *Streptococcus mutans*: *In silico* and *in vitro* study

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This study aims to evaluate the bacterial activity of Barangan peel against *Streptococcus mutans* (*S. mutans*) using *in silico* and *in vitro* methods. *In silico* conducted with AutoDock 4.0 evaluated ligand binding to GtfB (PDB ID: 3AIB), SwissADME, ProTox-II, and PASS online assessed pharmacokinetic, toxicity, and biological activity profiles. Antibacterial activity of Barangan peel at 10%, 20%, 35%, and 50% concentrations against *S. mutans* was determined using agar assays. The inhibition zones and colony count data were analyzed using one-way ANOVA ($p \leq 0.05$). Results showed Barangan peel phytochemical has low toxicity (Class 5–6, LD50 >2,000 mg/kg) and high biological potential for non-phenolic terpenoids (Pa=0.405). Cyclopropa stigmat steroid has the strongest affinities (−8.00 kcal/mol). The minimum inhibitory concentration (MIC) was at a 10% concentration, while the inhibition zone diameter and colony count showed significant differences ($p<0.05$) for all concentrations. Barangan peel phytochemicals exhibited favorable toxicity profiles and potent inhibitory activity against *S. mutans*.

Keywords: Banana, Antibacterial, *Streptococcus mutans*, Glucosyltransferase

INTRODUCTION

Dental caries continues to be an ongoing health issue in society, particularly in areas of poverty. The general health care system continues to prioritize dental and oral health, meaning oral care needs are not optimally served[1)]. The 2023 Indonesian Basic Health Research[2)] revealed that the prevalence of dental caries and sensitive teeth overall was 43.6% and 11.1%, indicating that oral and dental health in Indonesia has also not been given priority. Providing antibacterial or remineralization agents in mouthwash or toothpaste is one of the preventive efforts against dental caries.

Dental caries is a disease that requires a favorable environment to develop, including a fermentable carbohydrate diet, acid-producing bacteria (oral pathogens), and as a host, teeth and saliva. Among oral pathogens, *Streptococcus mutans* (*S. mutans*) is widely recognized as a primary contributor to dental caries due to its exceptional ability to form biofilms and produce acids that demineralize tooth enamel. The virulence of the bacteria is largely mediated by enzymes such as glucosyltransferases (Gtfs), which synthesize extracellular polysaccharides (EPS) essential for adherence and biofilm maturation. Targeting these enzymes represents a promising strategy to mitigate the cariogenic potential of *S. mutans*[3-5)].

The exploration of plant-derived compounds for antimicrobial activity has gained considerable traction. Banana (*Musa* spp.) peels, an abundant agro-waste, are emerging as a potential candidate due to their rich composition of bioactive phytochemicals, including polyphenols, flavonoids, tannins, and alkaloids, which have demonstrated antimicrobial, antioxidant, and anti-inflammatory properties in various studies[6)]. Banana peel extract (using ethanol and distilled water as solvents) at a minimum concentration of 3.125 mg/L has been reported to inhibit *S. mutans*. While the minimum killing threshold with ethanol solvent is 50 mg/mL and 100 mg/mL for distilled water solvent[7)]. Banana peels have antioxidant qualities due to their high catechin concentration (0.50–30 mg/L), making them non-toxic to human cells[8)].

The phytochemical and mineral composition of banana peels varies depending on the species and place of origin[8)]. Barangan (*Musa acuminata* Colla) is the typical banana of Medan, Sumatera Utara, Indonesia, and one of the main agricultural products. Barangan peel waste will increase with the amount of its production and processing. Utilizing banana peels can reduce organic waste, which accounts for 60% of the total waste in Medan[9)].

The *in silico* molecular docking method has become an indispensable computational tool in drug discovery, particularly for screening natural products. This method provides insights into binding modes, affinities, and the potential inhibitory mechanisms of candidate compounds by simulating the interactions between small molecules and target proteins[10)]. In the context of *S. mutans*, molecular docking can be employed to evaluate how

Received Jan 13, 2026: Accepted Feb 25, 2026
doi:10.4012/dmj.2026-010 JOI JST.JSTAGE/dmj/2026-010

bioactive molecules from banana peels might interact with key enzymes, such as Gtfs, thereby disrupting biofilm formation and reducing pathogenicity[11]. This *in silico* approach not only accelerates the identification of promising antimicrobial candidates but also lays the groundwork for subsequent *in vitro* and *in vivo* validations, ultimately contributing to the development of innovative, nature-based therapeutic strategies in dentistry[12].

The Kirby-Bauer disk diffusion method is frequently used as a main screening method because of its ease of use, affordability, and capacity to deliver quick qualitative insights into antibacterial activity. Broth dilution techniques are frequently used for a more thorough and quantitative evaluation to find the minimum inhibitory concentration (MIC), which is the lowest concentration of an agent that can prevent observable bacterial growth. The Clinical and Laboratory Standards Institute (CLSI, 2023) firmly supports this approach as the gold standard for antimicrobial susceptibility testing due to its repeatability and dependability[13]. The minimum bactericidal concentration (MBC), in addition to MIC, provides further information about the antimicrobial process by detecting the lowest dose that causes bacterial cell death.

The originality of this study resides in its translational, mechanism-based innovation of dental biomaterials by demonstrating that bioactive compounds derived from Barangan peel act as targeted inhibitors of glucosyltransferase B (GtfB) of *S. mutans*, and determining the precise dosage. This offers a legitimate anti-virulence strategy that can be incorporated into next-generation caries-preventive formulations. Therefore, the purpose of this study is to evaluate the bacterial activity of Barangan (*M. acuminata* Colla) peel against *S. mutans* using both *in silico* and *in vitro* methods.

MATERIALS AND METHODS

This study has been ethically approved by the Health Research Ethics Committee Universitas Sumatera Utara, Medan, Indonesia, No. 212/KEPK/USU/2024.

Preparation of Barangan peel powder

Ripe Barangan (*M. acuminata* Colla) were collected from Deli Serdang District, North Sumatra Province, Indonesia. Barangan peels were separated from the pulp, washed under running water, drained, and dried with a clean cotton towel. The peels were cut into small pieces and oven-dried at 60°C for 12 h. The dried material was ground using a chopper and sieved through a 100-mesh filter to obtain a uniform particle size. Further size reduction was carried out using a planetary ball mill (PM 200, Retsch, Haan, Germany) with 5 mm balls at 800 rpm for 1 h to produce fine peel powder.

Phytochemical screening gas chromatography–mass spectrometry (GC–MS) analysis

Five grams of Barangan peel powder were extracted with 100 mL of ethanol at room temperature for 48 h with occasional stirring. The mixture was filtered, and the extract was analyzed using GC–MS (Agilent 5977B GC/MSD, Agilent Technolgy, Santa Clara, CA, USA). The analysis was performed at LABKESDA DKI, Jakarta, Indonesia.

In silico molecular docking analysis

Molecular docking was performed with AutoDock 4.0 to evaluate the binding interactions of selected phytochemical ligands with the catalytic domain of GtfB from *S. mutans* (PDB ID: 3AIB)[11]. Toxicity profiles were assessed using the ProTox-II (ProTox-3.0) server, while biological activity predictions were carried out with PASS (Pass-GeneXplain). This combined *in silico* approach enabled evaluation of binding potential, biological activity, and safety profiles of candidate compounds.

Agar media, bacterial preparation and inoculation

Thirty-eight gram per litre Mueller–Hinton agar (MHA; CM0337, Oxoid, Basingstoke, UK) and 21 g/L Mueller–Hinton broth (MHB; CM0405B, Oxoid) were prepared in distilled water, boiled until homogeneous, and sterilized at 121°C and 2 atm for 15 min. Ten milliliters of MHA were poured into sterile petri dishes and allowed to solidify.

A colony of *S. mutans* ATCC® 25175™ was inoculated into 2 mL MHB and incubated at 37°C for 24 h in a shaker incubator (120 rpm). After incubation, 1 mL of culture was diluted in 9 mL of 0.85% NaCl until the turbidity matched the 0.5 McFarland standard (~1×10^6 CFU/mL), verified visually against the standard tube. The standardized suspension was used immediately for antimicrobial assays.

MIC and MBC

Different concentrations of Barangan peel powder (10%, 20%, 35%, and 50%) were prepared in distilled water. Fifteen Petri dishes containing 15 mL MHA were inoculated with *S. mutans* (≈10^6 CFU/mL). A sterile cotton swab was dipped into the bacterial suspension and evenly spread across the agar. Sterile paper discs impregnated with the solution, along with 0.2% chlorhexidine (positive control), were placed on the agar surface. Plates were incubated at 37°C for 24 h, and inhibition zones were measured using a digital caliper (Krisbow, Jakarta, Indonesia). The MIC was defined as the lowest extract concentration that produced a visible inhibition zone.

For MBC testing, tubes containing *S. mutans* suspension (10^6 CFU/mL) were incubated with extract concentrations at and above the MIC for 24 h at 37°C. After incubation, 1 mL broth from each tube was plated on plate count agar (PCA; CM0325, Oxoid), homogenized by gentle swirling, and incubated at 37°C for 24 h. The MBC was determined as the lowest concentration with no visible bacterial growth, confirmed using a colony counter.

Statistical analysis

All statistical analyses were performed using IBM SPSS Statistics version 25 (IBM, Armonk, NY, USA). The data, including the inhibition zone diameter (mm) and the number of colonies (CFU/mL), were statistically analyzed using a one-way ANOVA test ($p \leq 0.05$).

RESULT

Phytochemical screening, toxicity, and biological activity profiles

The phytochemical profiling of Barangan banana peels revealed diverse compounds with different groups, abundances, and predicted biological activities, as shown in Table 1. The most abundant compound was benzamide, N-(2-cyano-4,5-diethoxyphenyl)-4-fluoro- with a content of 38.84%, followed by 1-(2-hydroxypropan-2-yl)-3a-methyl-6,10-dimethylidene-decahydro-1H-cyclopenta[11]annulene-5,9-diol (24.14%) and cyclopropa[5,6]stigmast-22-en-3-one,3′,6-dihydro-(5.beta.,6.alpha.,22E)- (14.29%). A non-phenolic terpenoid derivative (4H-1,3-benzodioxin-4-one derivative) was also identified at 9.30%, while gamma sitosterol (2.51%), vitamin E (2.01%), and hexadecanoic acid, methyl ester (1.24%) were present in smaller proportions.

Based on PASS predictions, the non-phenolic terpenoid exhibited the highest probability of activity (*Pa*=0.405; *Pi*=0.029), followed by the polycyclic triterpenoid (*Pa*=0.386; *Pi*=0.038) and the steroid compound (*Pa*=0.203; *Pi*=0.114). The benzamide derivative, despite being the most abundant, demonstrated lower predicted activity (*Pa*=0.135; *Pi*=0.085). Predicted toxicity classifications ranged from class 5 to 6, with the majority of bioactive compounds falling into class 5, whereas the benzamide derivative was categorized as class 6. Compounds such as vitamin E, gamma sitosterol, and methyl ester hexadecanoic acid did not yield measurable PASS-predicted activity.

In silico molecular docking study

Molecular docking results showed the binding affinity value of the phytochemical component in Barangan peels with GtfB protein ligand of *S. mutans* (PDB ID: 3AIB) and its structure interaction is presented in Table 2 and Fig. 1. As a result, the Barangan peels compounds of the steroid group, cyclopropa[5,6]stigmast-22-en-3-one,3′,6-dihydro-(5.beta.,6.alpha.,22E)-, show the greatest binding affinity compared to other phytochemical components, with a binding affinity value of −8,70 kcal/mol. While the binding affinity of chlorhexidine, used as a positive control, is −9.90 kcal/mol.

Chlorhexidine as the positive control exhibited the highest binding affinity to GtfB supported by diverse interactions including π-anion, salt bridge, hydrogen bonding, and π–π stacking with key catalytic residues (Fig. 1a). The Barangan peels compound, cyclopropa[5,6]stigmast-22-en-3-one,3′,6-dihydro-(5.beta.,6.alpha.,22E)-, relied predominantly on hydrophobic interactions, including π-alkyl and van der Waals with nonpolar residues (Fig. 1b). Other compounds, such as C(14a)-Homo-27-nor-14β-gammaceran-3α-ol and 11-(2-Hydroxypropan-2-yl)-3a-methyl-6,10-dimethylidene-2,3,4,5,7,8,9,11,12,12a-decahydro-1H-cyclopenta[11]annulene-5,9- diol, showed only modest affinities (−1.36

Table 1 Phytochemical components, prediction of toxicity profiles and biological activity of Barangan (*M. acuminata* Colla) peel

Phytochemical compound	Molecular formula	Group	Content (%)	Predicted toxicity	Biological activity	
					Pa	*Pi*
Hexadecanoic acid, methyl ester	$C_{17}H_{34}O_2$	Palmitic acid	1.24	—	—	—
Vitamin E	$C_{29}H_{50}O_2$	Trepene-derived	2.01	—	—	—
Gamma Sitosterol	$C_{29}H_{50}O$	Phytosterol	2.51	—	—	—
1-(2-Hydroxypropan-2-yl)-3a-methyl-6,10-dimethylidene-2,3,4,5,7,8,9,11,12,12a-decahydro-1H-cyclopenta[11]annulene-5,9-diol	$C_{20}H_{34}O_3$	Polycyclic triterpenoid	24.14	5	0.386	0.038
4H-1,3 - Benzodioxin-4-one, 2-(1,1-dimethylethyl) hexahydro -5- methyl -4a-(2-propenyl)-,[2s-(2.alpha., 4a.alpha.,5.beta.,8a.beta.])	$C_{16}H_{26}O_3$	Non-phenolic terpenoid	9.30	5	0.405	0.029
Benzamide, N-(2-cyano-4,5-diethoxypheny)-4-fluoro-	$C_{15}H_{14}FNO_3$	Benzamide	38.84	6	0.135	0.085
Cyclopropa[5,6]stigmast-22-en-3-one,3′,6-dihydro-(5.beta.,6.alpha.,22E)-	$C_{30}H_{48}O$	Steroid	14.29	5	0.203	0.114

Table 2 Binding affinity value of specific phytochemical ligands of Barangan (*M. acuminata* Colla) peel and the catalytic domain of GtfB from *S. mutans* (PDB ID: 3AIB)

No.	Compound	Binding affinity
1	Chlorhexidine (commercial drugs)	−9.90
2	Benzamide, N-(2-cyano-4,5-diethoxypheny)-4-fluoro-	1.19
3	1-(2-Hydroxypropan-2-yl)-3a-methyl-6,10-dimethylidene-2,3,4,5,7,8,9,11,12,12a-decahydro-1H-cyclopenta [11] annulene-5,9-diol	−1.67
4	Cyclopropa[5,6]stigmast-22-en-3-one,3′,6-dihydro-(5.beta.,6.alpha.,22E)-	−8.70
5	C(14a)-Homo-27-nor-14.beta.-gammaceran-3.alpha.-ol	−1.36
6	4H-1,3-Benzodioxin-4-one, 2-(1,1-dimethylethyl) hexahydro-5-methyl-4a-(2-propenyl)-,[2s-(2.alpha.,4a.alpha.,5.beta.,8a.beta.])	4.27

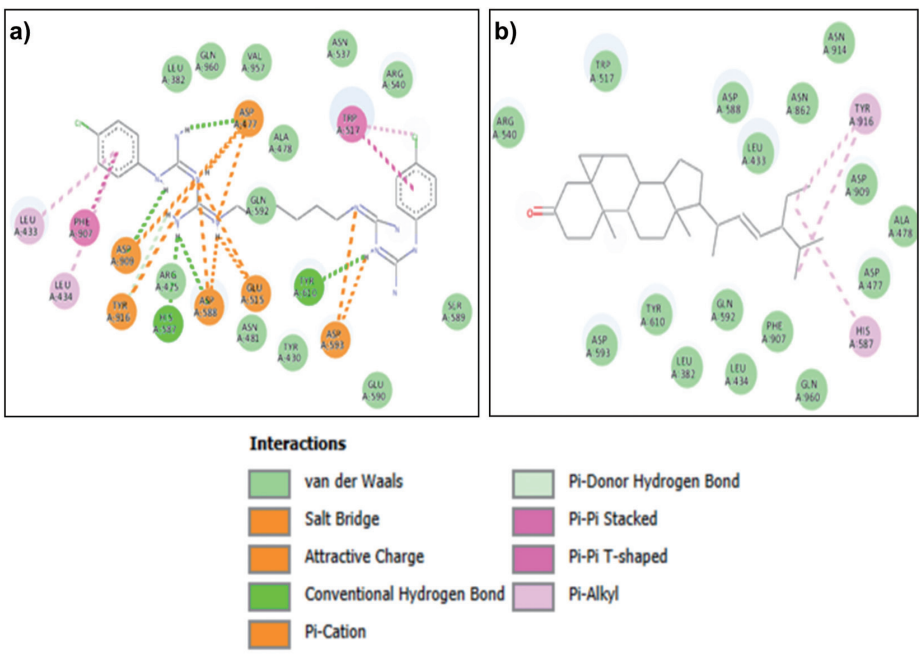

Fig. 1 Schematic molecular structure interaction (high binding affinity) between specific phytochemical ligands and the catalytic domain of GtfB from *S. mutans* (PDB ID: 3AIB).
a) Chlorhexidine; b) cyclopropa[5,6]stigmast-22-en-3-one,3′,6-dihydro-(5.beta., 6.alpha.,22E)- of Barangan (*M. acuminata* Colla) peel.

and −1.67 kcal/mol), while benzamide,N-(2-cyano-4,5-diethoxyphenyl)-4-fluoro and the benzodioxin derivative yielded positive binding energies (+1.19 and +4.27 kcal/mol), indicating poor or unstable binding under the docking conditions[14-16].

MIC and MBC

The antibacterial activity of Barangan peel is demonstrated by the formation of inhibition zones on agar media as shown on Fig. 2. The inhibition zone diameter results showed in Table 3 indicate that the Barangan peels solution at 50% concentration exhibited the largest inhibition zone (24.33±0.15 mm), followed closely by the positive control at 24.17±0.29 mm, and the other concentrations of 35%, 20%, and 10%, which measured 22.53±0.21 mm, 13.8±0.10 mm, and 10.47±0.15 mm, respectively. Moreover, the one-way ANOVA test ($p \leq 0.05$) revealed significant differences in the inhibitory zones between the control group and the 10%, 20%, and 35% Barangan peel groups. Meanwhile, the control group and the 50% Barangan peels group exhibited no significant differences. This study revealed that the MIC of the Barangan peels solution is at 10% concentration.

The number of colony data (Table 3) showed that there are no significant differences between all groups,

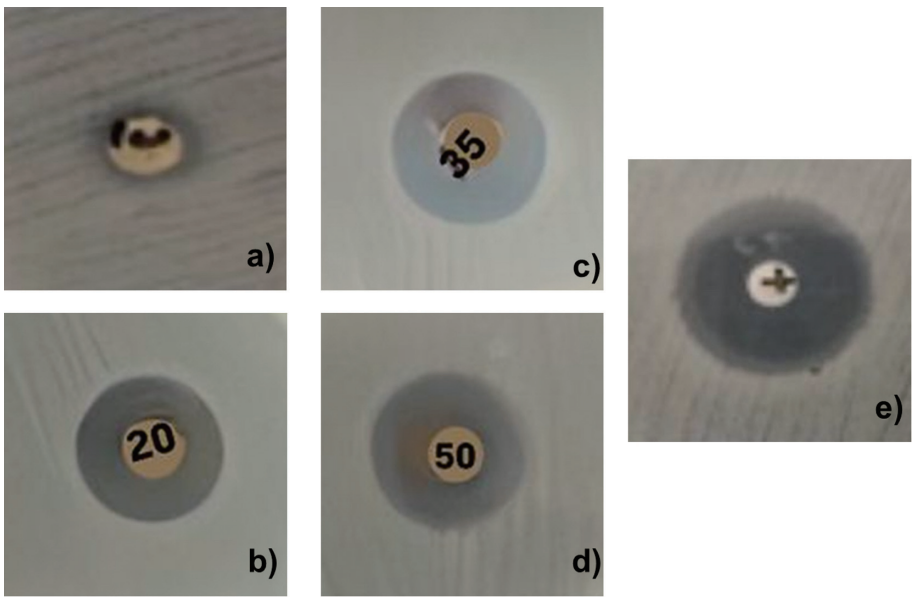

Fig. 2 Representative of inhibition zone from agar media: Barangan (*M. acuminata* Colla) peel solution.
a) 10%; b) 20%; c) 35%; d) 50%; and e) positive control (Chlorhexidine 0.2%).

Table 3 Mean value (SD) of inhibition zone diameter and colony count at various concentrations of Barangan (*M. acuminata* Colla) peel solution against *S. mutans* ATCC® 25175™

Treatment group		Inhibition zone diameter (mm)	Number of colony (CFU/mL)	Reduction (%)
Barangan Peel	10%	10.47 (0.15)[a]	1724.67 (66.03)	64.94
	20%	13.80 (0.10)[a]	63.33 (13.5)[b]	98.71
	35%	22.53 (0.21)[a]	6.67 (4.73)[b]	99.86
	50%	24.33 (0.15)[a,b]	0[b]	100
Chlorhexidine (Positive control)	0.2%	24.17 (0.29)[a,b]	0[b]	100

[a] significant differences ($p<0.05$) between groups (One way ANOVA with *post hoc* LSD $p\leq0.05$)
[b] no significant diffrences ($p>0.05$) between groups (One way ANOVA with *post hoc* LSD $p\leq0.05$)

except for the 10% Barangan peels Group. Chlorhexidine and 50% Barangan peels result in a 100% decrease in colonies and 0 CFU/mL.

DISCUSSION

Development of dental caries is multifactorial, resulting from the complex interplay of biological, environmental behavioral factors, and is related to oral microbiota alteration. *S. mutans* is recognized as the primary etiological agent due to its ability to produce in–rich EPS and a low-pH milieu, which can alter the human oral environment and establish a pathogenic niche for acidogenic and aciduric bacteria. *S. mutans* synthesized EPS through Gtfs, which regulate the formation of dental plaque by constructing a structural framework for biofilm organization. This framework facilitates strong bacterial adhesion and enhances the stability of biofilm on the tooth and bacterial cells[3,14].

Phytochemical analysis of Barangan peel revealed a rich composition dominated by a benzamide derivative (38.84%), followed by a polycyclic triterpenoid (24.14%) and a steroid derivative (14.29%). In addition, a non-phenolic terpenoid was present at 9.30%, while γ-sitosterol, vitamin E, and hexadecanoic acid, methyl ester, accounted for smaller proportions. These findings align with previous reports that banana peel contains high levels of terpenoids, tannins, and flavonoids, which contribute to their antimicrobial activity and antioxidant potential[6,17].

To assess drug safety, toxicity profiles were predicted using ProTox-II and biological activity with PASS Online. The result of this study (Table 1) indicates that the majority of the chemicals were classified as toxicity class 5, suggesting they may be harmful if swallowed but are less acutely toxic than those in classes 1–4.

Benzamide was classified as class 6, reflecting non-toxic behavior under acute oral exposure conditions. This makes benzamide structurally safe, despite its weak docking score. No strong hepatotoxicity, mutagenicity, carcinogenicity, or cytotoxicity flags were reported in ProTox-II for the leading compounds[18].

The PASS predictions suggest that terpenoid and triterpenoid chemicals, especially non-phenolic terpenoids and polycyclic triterpenoids, are the most potent bioactive elements in Barangan peels. Their moderate to high *Pa* values, along with tolerable safety profiles, indicate potential usefulness as antibacterial agents. Therefore, while the compounds may not act as potent drugs individually, they may exhibit multi-target or additive effects, especially when considered as part of a crude extract or phytochemical mixture. Notably, the compound with the strongest binding score (cyclopropa stigmat steroid) also had favorable toxicity (class 5) and a moderate activity prediction (*Pa*=0.203), suggesting potential as a lead compound for further *in vitro* validation and potential modification to enhance activity. These structural classes are extensively validated in the literature for oral health applications. Plant-derived compounds, specifically terpenes and flavonoids, exhibit antibacterial and anti-biofilm properties comparable to those of chlorhexidine and present promising potential in strategies aimed at preventing dental caries[19,20].

Moreover, *in silico* molecular docking was used to assess the binding affinity of certain phytochemicals extracted from Barangan peels towards the catalytic domain of GtfB from *S. mutans* (PDB ID: 3AIB). Binding affinities were expressed in kcal/mol, with more negative values indicating stronger predicted interactions[11]. The docking studies indicate that phytochemicals extracted from Barangan peel exhibit substantial binding affinities for GtfB, comparable to those of chlorhexidine. Surprisingly, the majority of cyclopropa's interactions are hydrophobic, suggesting a nonpolar binding mode that may be related to an allosteric or membrane-mimetic mechanism[21,22]. This supports findings of tannic acid and other tiny hydrophobic compounds with significant Gtf-binding affinities[20,23-25].

Despite its high abundance, the benzamide derivative presented low expected activity, showing that quantity in the extract does not correlate with functional significance and emphasizing the necessity for focused computational and empirical screening. Meanwhile, the steroid derivative's moderate activity might suggest alternative mechanisms of action, in line with findings that hydrophobic small molecules can modulate microbial enzyme functions *via* non-polar interactions[26]. Although vitamin E and γ-sitosterol did not present significant predicted activity, literature supports their antioxidant and membrane-stabilizing roles, which could contribute synergistically to antimicrobial effects[17]. The phytochemicals in Barangan peel may offer versatile anti-cariogenic strategies with reduced toxicity compared to traditional antimicrobials by targeting GtfB through several binding methods, including direct occupation of the active site or insertion into hydrophobic pockets[22].

These *in silico* results were supported by the *in vitro* test of the antibacterial effect of Barangan peel. The antibacterial effect of Barangan peel solution is attributed to its bioactive compounds. The near-equivalence in inhibition zones between the 50% Barangan peel solution and 0.2% chlorhexidine suggests that phytochemical synergy at high concentrations may overcome the potency gap between natural and synthetic antimicrobials. The solution has diminished efficacy at lower concentrations, indicating that its antibacterial action is constrained by dosage. This is consistent with earlier research on banana peel that showed better antimicrobial activity at higher levels[7]. Chlorhexidine demonstrated complete inhibition (100%), confirming its strong bactericidal property but also highlighting its well-documented drawbacks, such as disruption of the commensal oral microbiota and potential cytotoxicity when used long-term[27,28].

Meanwhile, this study also revealed that Barangan peels solution at lower concentrations (20% and 35%) effectively reduced bacterial counts but did not fully eliminate all colonies. This outcome is consistent with the ecological concept that oral antibacterial agents should not aim for complete eradication of microorganisms, as total suppression of the oral microbiome may disrupt microbial homeostasis and lead to dysbiosis[27-29]. Instead, the therapeutic goal is to suppress pathogenic bacteria while maintaining beneficial species essential for oral health. This emphasises the benefit of natural agents such as Barangan peels, which demonstrate considerable antibacterial properties without completely eradicating microbial populations, thereby fitting more closely with an ecological approach to caries care.

The results support the concept that plant-based extracts, when properly concentrated, can match the efficacy of traditional antiseptic agents, particularly when combined with complementary processes such as enzyme suppression and biofilm breakdown. Moreover, Barangan peel, which is rich in terpenoids and triterpenoids, in low concentration, provide structural support that might be able to lessen the virulence of *S. mutans*, a significant dental caries-causing bacterium.

CONCLUSION

Barangan (*M. acuminata* Colla) peel contains bioactive phytochemicals with safe toxicity profiles and strong predicted antibacterial potential. Molecular docking demonstrated that the cyclopropastigmat steroid from Barangan peels exhibits high-affinity interactions with GtfB of *S. mutans*, validated by MIC and MBC experiments that proved substantial antibacterial activity. These findings suggest 50% Barangan peel solution has the same antibacterial effect as 0.2% chlorhexidine. Lower concentrations have also shown a decrease in the virulence of *S. mutans* and are thus viewed as a feasible natural option for oral hygiene formulations designed to prevent the development of biofilms and cariogenic bacteria. Further study will be needed to translate these findings into practical dental

applications, encompassing *in vivo* validation and clinical formulation studies.

ACKNOWLEDGMENTS

The author thanks Dr. Diana Setyaningsih and the team from Universitas Syiah Kuala, Banda Aceh, Indonesia, for their contribution to the molecular docking analysis.

CONFLICT OF INTEREST

The authors declare no conflict of interest.

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