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Penulis : **Meiny Faudah Amin**, Dikdik Kurnia, Taufiq Ariwibowo, Dicky Hardy

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Dr Anne Agustina Suwargiani, drg, MKM, <jurnal.fkg@unpad.ac.id>
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Jul 28, 2025, 3:12 PM



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Meiny Faudah Amin

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ORIGINAL ARTICLE

Multi-Target Potential of *Moringa oleifera*-Derived Compounds against cariogenic and Endodontic Virulence Proteins by Molecular Docking Analysis Reveals; Research Article

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ABSTRACT

Introduction: Dental infections, including cariogenic and endodontic conditions, are multifactorial diseases, including bacterial adherence, biofilm formation, and tissue damage. Furthermore, genetics, as well as environmental and behavioral factors, influence disease onset, susceptibility, and progression rate. The progression of the disease and its clinical manifestations are caused by the interaction between the host immune system and the bacteria found in dental plaque. Potential substitutes for current antibiotics are being studied, including natural compounds with broad-spectrum antibacterial properties. *Moringa oleifera*, a medicinal plant that has long been used to treat systemic and oral diseases, is one of the natural sources. [This study aimed to systematically evaluate the interaction profiles of four *Moringa oleifera*-derived compounds against multiple virulence-associated proteins of key cariogenic and endodontic pathogens using in silico molecular docking.] **Methods:** This study was conducted by molecular docking simulations to assess the binding energy of four *M. oleifera*-derived compounds-eugenol, trans-anethole, arachidonic acid, and phytosphingosine-to five important virulence-associated proteins from key cariogenic and endodontic pathogens of Cystalytin, SrpA, FimA, RadD, and Ddl. AutoDock 4.0 was utilized in docking simulations. **Results:** Phytosphingosine-Ddl exhibited the lowest binding energy of -7.42 kcal/mol, followed by eugenol with three different receptors-Cystalytin, SrpA, and FimA-and arachidonic acid-RadD. The lowest inhibition constant was shown by the phytosphingosine-Ddl complex of 3.61 μ M. Each compound interacted with various targets, but phytosphingosine exhibited the most consistent and widespread predicted binding via hydrogen bonds of Glu222, Arg291, Glu306, Asp293, Lys251, and hydrophobic interactions of Phe295, Phe245, Phe175, and Leu145. **Conclusion:** These findings demonstrate that phytosphingosine can disrupt multiple virulence processes, highlighting its potential as a supplementary therapeutic agent in conservative dentistry.

KEYWORDS

Molecular Docking, *Moringa oleifera*, Periodontitis, Cariogenic pathogens, Virulence factors

INTRODUCTION

An inflammatory condition caused by infection that affects the hard and soft tissues of the tooth—such as enamel, dentin, pulp, and periapical tissues—is characteristic of various dental diseases in the field of conservative dentistry, including cariogenic and endodontic infections¹. Furthermore, the development of

Reviewer ...

The manuscript addresses a relevant topic and presents a clear multi-target molecular docking screen of four *Moringa oleifera*-derived compounds against five oral pathogen virulence proteins. The idea is sound and the docking

Mainy F Amin

Thank you for your helpful comments. We have revised the manuscript accordingly. Technical errors have been corrected, and additional methodological details—including docking parameters, validation steps, and

Reply

Reviewer ...

Add type of research

Mainy F Amin

Thank you for the suggestion. We have added the type of research

Reply

Reviewer ...

state the research objectives here;

Mainy F Amin

Thank you for the helpful comment. We have added a clear statement of the research objectives

Reply

Reviewer ...

Please make sure, this is for periodontitis or cariogenic or endodontics

Mainy F Amin

Thank you for the comment. We have clarified the disease focus in the revised manuscript. While most virulence proteins (Cystalytin, FimA, RadD, and SrpA) are derived from periodontitis-related pathogens, Ddl

Reply

Reviewer ...

the disease, the exposure of vulnerable individuals to its onset, and the rate of advancement are all influenced by genetics as well as environmental and behavioral variables. Multiple factors contribute to the aetiology of periodontitis². In a vulnerable host, subgingival dental biofilm triggers an inflammatory and immunological reaction that ultimately results in the irreversible destruction from dental tissue to the periodontium, which includes the alveolar bone and periodontal ligament³. Subgingival bacteria, their virulence factors, and host immunological responses combine intricately to cause irreversible damage, pulp necrosis and periodontitis, a multifactorial inflammatory disease. The formation of organized, multispecies biofilms and the coordination of diverse bacterial tactics to colonize, persist, and harm periodontal tissues are important aspects of disease progression⁴.

These various virulence mechanisms are demonstrated by a number of proteins from common oral pathogens: RadD, an adhesin necessary for interspecies coaggregation and expressed by *Fusobacterium nucleatum*, links early and late colonizers in the dental plaque matrix to promote the production of complex biofilms⁵. The serine-rich repeat adhesin SrpA, which is produced by *Streptococcus sanguinis*, binds salivary glycoproteins and facilitates early bacterial adhesion to tooth surfaces and other microorganisms, starting the formation of biofilms⁶. To adhere to host epithelial cells, invade oral tissues, and co-aggregate with other pathogenic bacteria to sustain mature biofilms, *Porphyromonas gingivalis* utilizes FimA, a key fimbrial protein⁷. *Streptococcus mutans* D-alanine: D-alanine ligase (Ddl) is a key enzyme in the biosynthesis of peptidoglycans, preserving the integrity of the bacterial cell wall, allowing for survival in the oral cavity's acidic and immunologically demanding environment, and indirectly promoting biofilm stability by preserving bacterial viability⁸. Finally, the PLP-dependent L-cysteine desulfhydrase Cystalytin, which is secreted by *Treponema denticola*, breaks down host cysteine to produce hydrogen sulfide and ammonia. These substances harm epithelial cells, disrupt tissue barriers, and trigger inflammatory responses that contribute to the degradation of dental and surrounding oral tissues⁹.

More research is being conducted on natural substances with broad-spectrum antimicrobial activities as potential substitutes for existing antibiotics, particularly those that target bacterial virulence rather than viability. Promising candidates include phytosphingosine, arachidonic acid, trans-anethole, and eugenol-bioactive compounds that have been shown to have antibacterial, anti-inflammatory, and biofilm-disrupting qualities¹⁰⁻¹². The structures of the compound were presented in **Figures 1**. However, *Moringa oleifera*, a medicinal plant that has long been used to treat systemic and oral infections, contains all four of these compounds^{14, 15}. All the compounds were found in the extract based on the data of the extract's LC-MS analysis. The application of compounds produced from *M. oleifera* is consistent with new approaches to managing periodontitis, which seek to reduce the development of antibiotic resistance while interfering with bacterial virulence factors and biofilm formation^{16, 17}.

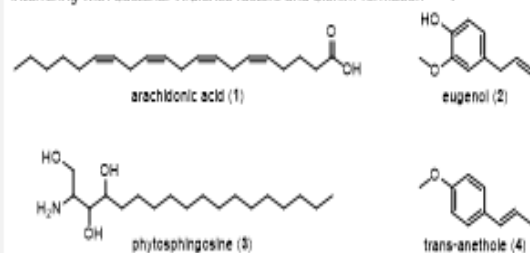


Figure 1. Structure of *Moringa oleifera* derived compounds

Reviewer

Please complete it for an example you can see the previous PID publication

Meiny F Amin

Thank you, we have added it

Comprehensive studies assessing the efficacy of natural compounds against key virulence factors involved in cariogenic and endodontic infections remain limited, despite growing interest in these compounds as alternative antimicrobial agents. Four compounds derived from *M. oleifer*, eugenol, *trans*-anethole, arachidonic acid, and phytosphingosine, are evaluated simultaneously against a selected group of five virulence-associated proteins from major oral bacteria. These proteins of Cystalylin, FimA, Ddl, SrpA, and RadD represent various mechanisms of adhesion, biofilm formation, cell survival, and tissue destruction.

The novelty of this study lies in the simultaneous multi-target evaluation of these four natural compounds against virulence-related proteins, an approach that has not been reported previously. This study aims to ascertain the binding affinities and predict the interaction profiles of these natural compounds, identify the compounds with the strongest potential to inhibit multiple virulence targets, and provide computational evidence supporting further exploration of *M. oleifer* constituents as adjuvant agents in the prevention and treatment of periodontitis using molecular docking simulations.

METHODS

The *in silico* method was employed to conduct the research, which involved molecular docking simulations to determine the molecular activity of each compound towards specified receptors. The three-dimensional structures of each receptor were obtained from the RCSB Protein Data Bank website (<https://www.rcsb.org/>). This study used five receptors: Cystalylin (PDB ID: 1C70), SrpA (PDB ID: 5EQ3), FimA (PDB ID: 6JZK), RadD (PDB ID: 7R7J), and Ddl (PDB ID: 7U9K). Two reference ligands were used for each target protein: the native ligand and a positive control. The native ligand refers to the biological ligand that was crystallized together with the protein in the PDB structure, representing the natural binding conformation within the active site. The positive control refers to an inhibitor or compound that has been previously reported to interact with the corresponding target protein, and is included to provide a reference for comparison with the docking performance of the tested phytochemical compounds. L-arginine for RadD, D-glycoserine for Cystalylin and Ddl, Neu5Gc for SrpA and GalNAc for FimA were the three positive controls utilized in this study. All of the structures were obtained from PubChem with CIDs 67427, 440001, 6234, and 35717. Four compounds-arachidonic acid, eugenol, phytosphingosine, and *trans*-anethole-found in *M. oleifer* were examined for their capacity to interfere with virulence factors of periodontitis. The structures of arachidonic acid, eugenol, phytosphingosine, and *trans*-anethole were obtained from the PubChem website (<https://pubchem.ncbi.nlm.nih.gov/>) with CIDs of 444899, 3314, 122121, and 637563, respectively. After downloading each ligand structure in SDF format, they were all converted to pdb format and optimized using Chem3D Ultra 12.0's MM2 energy minimizer. To validate the docking protocol, we re-docked each original ligand to its respective protein binding site after removing it from the original crystal structure. The root mean square deviation (RMSD) between the docking pose and the crystallographic pose was calculated to assess the reliability of the docking setup. An RMSD value < 3.0 Å was considered acceptable, indicating that the selected docking parameters were able to accurately reproduce the experimentally observed binding conformation. The RMSD re-docking values are obtained in **Table 1 and Figure 2**.

Table 1. Grid center coordinates for each receptor

Receptor's name	PDB ID	Positive Control	Grid Center (coordinates)			RMSD
			x	y	z	
Cystalylin	1C70	D-glycoserine	14.561	-4.847	20.75	2.167
SrpA	5EQ3	Neu5Gc	15.260	11.538	9.568	2.436
FimA	6JZK	GalNAc	1.287	-3.755	93.007	3.102

Reviewer ⋮ ✎ 📄

The Introduction should clearly identify the novelty of this research (e.g., "The novelty of this research lies in..."), explaining how it contributes new insights or

Mainy F Amin

Thank you for the valuable feedback. We have revised the Introduction accordingly. The updated version now clearly states the novelty of this research by explicitly describing how our multi-target molecular docking

Reply

Reviewer ⋮ ✎ 📄

The manuscript mixes "native ligand" and "positive control" terms. Define each and explain selection (e.g., D-cycloserine for Ddl, GalNAc for FimA). Show re-docking RMSD of native ligand to validate docking setup and report

Mainy F Amin

Thank you for this valuable comment. We have performed the re-docking validation for all native ligands. Most ligands produced RMSD values below 2.0 Å, indicating good agreement with the

Reply

Reviewer ⋮ ✎ 📄

Please add the positive control for SrpA

Mainy F Amin

Thank you for the comment. The positive control for SrpA has been added.

Reply

Reviewer ⋮ ✎ 📄

Please check again. The grid center for Cystalylin lists y = -4847 which is almost certainly a typographical or copy paste error. Verify and correct all grid center coordinates and units (Å). Report the grid box origin consistently with

RadD	7R7J	L-Arginine	-6.627	-37.876	107.279	3.097
Ddl	7U9K	D-galactosamine	7.923	20.387	27.732	1.159

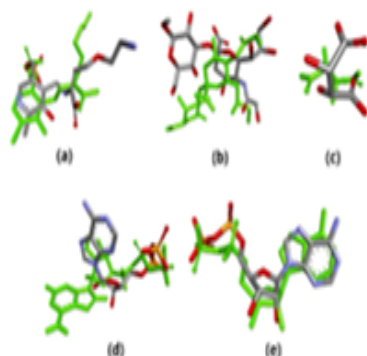


Figure 2. Re-docking conformation for (a) Cystalyzin, (b) SrpA, (c) FimA, (d) RadD, and (e) Ddl.

The AutoDock 4.0 application was used to carry out the molecular docking simulations. Every receptor and ligand in PDB format was converted to pdbqt format before the simulations commenced. For every receptor, a 40 Å x 40 Å x 40 Å grid box was applied, featuring specific x, y, and z coordinates of the grid center. Each receptor's coordinates were provided in **Table 1**. All of the receptors were subjected to a 0.375 Å spacing. The binding energy and inhibition constant for every receptor-ligand complex were analyzed. Using Discovery Studio 2020, each receptor-ligand complex's interaction was examined and illustrated. A graphic was created to illustrate the hydrophobic and hydrogen bonding interactions of receptor-ligand interactions.

RESULTS

The four compounds derived from *M. oleifera* showed different affinities for the five target proteins according to molecular docking simulations. The lowest (i.e., strongest) binding energies were typically displayed by the native ligands, with RadD (-8.27 kcal/mol) and Ddl (-8.94 kcal/mol) being especially remarkable. Eugenol showed consistently favorable binding energies across the majority of targets among the investigated natural compounds (-5.64 to -3.46 kcal/mol), followed by *trans*-anethole (-5.17 to -3.61 kcal/mol) and arachidonic acid (-5.13 to -1.73 kcal/mol). The most deprived binding was found for phytosphingosine, particularly with FimA (-1.74 kcal/mol) and SrpA (-2.68 kcal/mol). Positive controls demonstrated varied binding, with RadD (-2.78 kcal/mol) performing least favorably and Ddl (-6.09 kcal/mol) performing the best. Similar patterns were seen in calculated inhibition constants. Across all targets, the compounds showed K_i values in the nanomolar to millimolar range; native ligand binding to RadD (0.89 $\times 10^3 \mu\text{M}$ or 890 nM) and Ddl (0.28 $\times 10^3 \mu\text{M}$) had the lowest (strongest) K_i . However, the K_i values of the compounds were higher (weaker) than those of their respective positive controls for a number of targets, particularly SrpA and FimA. 54.29 $\times 10^3 \mu\text{M}$ or 54.29 mM for arachidonic acid binding to SrpA and 53.30 $\times 10^3 \mu\text{M}$ for phytosphingosine binding to FimA. The inhibition constants of each complex ligand and receptor were presented in **Table 2**.

Table 2. Molecular docking summary for all ligand-target pairs

Target	Ligand	ΔG	K_i	hydrogen bonds	hydrophobic interactions
Cystalyzin	Native	-6.78	10.76	Val98, Ala243, Tyr123, Ser237, Cys171, Lys238	-
	Positive control	-6.21	180.85	Arg368, Tyr124, Asp385, Glu30	-

Reviewer

Please add information in detail:

- State AutoDock Vina version and exact command / exhaustiveness used.
- Describe receptor preparation steps: how were missing

Mainy F Amin

Thank you for the comment

- In our study, we did not use AutoDock Vina; instead, the docking simulations were performed using AutoDock 4.0. Therefore, the Vina version and

Reply

Missing content

This comment thread contains content that's not yet supported. Select it to view it in the Revisions pane.

Reviewer

Please Reformat Tables 2–5 to include one line per ligand-target pair with columns: ΔG (kcal-mol⁻¹), computed K_i (nM or μM), number H bonds, key interacting residues, and whether interactions overlap native ligand

Mainy F Amin

Thank you for the suggestion. Tables 2–5 have been reformatted as requested.

Reply

	Comp. (1)	-5.13	174.80	Lys238, Tyr123	Cys171, Val99, Val98, Ala39, His206, Ile205, Val38, Ala243
	Comp. (2)	-5.64	72.98	Lys238, Tyr123, Phe206	Ala39, Ile205
	Comp. (3)	-3.81	1620	Ala39, Tyr123, Tyr124	Val99, Val98, Ile205, His206, Lys238, Ala238
	Comp. (4)	-5.17	161.76	Ala39, Tyr123, Asp385, Tyr124	Ala39, Cys171, Ile205, His206
SepA	Native	-6.36	21.70	Thr346, Gln344, Pro315, Tyr368, Arg347	Pro337, Arg342
	Positive control	-5.82	53.74	Arg342, Arg347, Thr346, Gln344, Tyr368, Ala343	-
	Comp. (1)	-1.73	54.26x10 ²	Arg342	Pro337, Phe294
	Comp. (2)	-4.22	802.41	Arg347, Thr346	Phe345, Gln344
	Comp. (3)	-3.18	4.663x10 ²	Gln344, Arg347, Thr346	Phe345, Pro347, Arg342
	Comp. (4)	-3.78	1.69x10 ²	Thr346	Arg342, Gln344
FlmA	Native	-4.96	230.57	Lys69, Thr61, Ser75, Met103	-
	Positive control	-4.73	343.094	Gly101, Asn100, Met103, Leu105, Val106	-
	Comp. (1)	-3.97	1.230	Lys69, Ser75	Lys108, Val106, Leu105
	Comp. (2)	-4.19	845.62	Met103	Ile71, Leu105
	Comp. (3)	-1.74	53.3x10 ²	Glu104, Val206	Ile71, Leu105
	Comp. (4)	-4.04	1090	Ser75	Leu105, Val106, Ile71
RadD	Native	-8.27	0.89 x10 ⁴	Arg343, Arg6, Tyr195, Gly36, Gly34, Ala33, Thr33	Arg343, Leu344
	Positive control	-2.78	9230	Asp315, Tyr195, Gly34, Arg6	-
	Comp. (1)	-4.68	390.63	Lys37, Thr33	Lys68, Arg6, Leu39, Leu37
	Comp. (2)	-4.00	1170	Gly36, Lys37	Ala35
	Comp. (3)	-2.67	11.12x10 ⁴	Gly34, Arg6, Tyr195, Leu344	Leu39, Leu37, Ala71, Lys37, Lys68
	Comp. (4)	-4.42	579.42	Gly34, Pro32	Leu39, Leu37, Lys68, Lys37, Ala35
Ddl	Native	-8.94	0.28 x10 ⁴	Lys130, Asn305, Glu213, Val216, Gln214, Glu220, Tyr246, Ser184, Gly182, Asn308, Ser183, Lys251	-
	Positive control	-6.00	34.60	Ile221, Phe294, Asn305, Glu222	-
	Comp. (1)	-6.52	16.40	Asn305	Leu145, Val216, Phe293, Phe175, Phe245, Ile187
	Comp. (2)	-5.40	109.80	Ala238, Ala244, Glu220	Phe293, Phe175, Leu145
	Comp. (3)	-7.42	3.61	Glu222, Arg291, Glu306, Asn293, Lys251	Phe293, Phe243, Phe175, Leu145
	Comp. (4)	-5.25	142.83	Phe245, Tyr246	Phe175, Phe293, Leu145

The *M. oleifera* compounds formed multiple hydrogen bonds across several targets, stabilizing their binding in active or binding sites. The native ligand-Ddl complex showed the most hydrogen bonds among other complexes, consisting of Lys130, Asn305, Glu213, Val216, Gln214, Glu220, Tyr246, Ser184, Gly182, Asn308, Ser183, and Lys251. Among the compounds, phytosphingosine formed strong hydrogen bonds, with phytosphingosine-Ddl presenting the most hydrogen bonds compared to other receptors, with residues Glu222, Arg291, Glu306, Asp293, and Lys251. Hydrophobic interactions were most abundant for arachidonic acid and phytosphingosine, which engaged numerous hydrophobic residues across targets, including Cys171, Val99, Val98, Ala39, His206, Ile205, Val38, Ala243 for arachidonic acid binding to Cystalyisin and Val99, Val98, Ile205, His206, Lys238, and Ala235 for phytosphingosine binding to Cystalyisin.

DISCUSSION

This study explores *Moringa oleifera*-derived compounds as potential multi-target inhibitors of key proteins involved in various stages of cariogenic and endodontic pathogenesis. Molecular docking and in-depth study of hydrogen bonding and hydrophobic interactions to determine how these compounds might interfere with adhesion-related receptors, enzymes required for bacterial survival,



Reviewer ⋮ ✎ 📄

Describe the results obtained from the research. The author compiles, analyzes, evaluates and interprets and compares the latest findings with findings

Moiny F Amin

Thank you for the valuable comment. The Discussion section has now been thoroughly revised. We have expanded the paragraphs, added deeper analysis and interpretation of the findings

and factors that contribute to host tissue damage. The results offer new insights into the ability of *M. oleifera* compounds to disrupt multiple virulence mechanisms relevant to dental infection progression, highlighting their potential as supplementary agents in comprehensive conservative dental therapy^{18, 19}.

Interaction potential of four compounds derived from *Moringa oleifera* extract against key virulence-associated proteins of cariogenic and endodontic pathogens. Scoring functions are used by docking programs to estimate this binding energy²⁰. A binding energy, a numerical depiction of the interaction between a ligand and a protein, can be estimated by molecular docking software. The sensitivity of various scoring functions to various kinds of interactions (such as hydrophobic and hydrogen bonding interactions) may vary. Higher binding affinities are generally indicated by lower (more negative) binding energies, which also imply a more stable and favorable interactions^{21, 22}. According to the docking data, almost all test ligands form 2–4 hydrogen bonds, mainly with key residues such as Lys238, Tyr123, His206, Ala39, and Val99. These residues are part of the same binding pocket as the native ligand, so the interaction of the test ligand can be said to overlap with the physiological binding site. This overlap indicates that the ligand is able to inhibit the proteolytic activity of Cystalytin through direct competition with the natural ligand. The greater the number of H-bonds, the more stable the interaction, and this is consistent with the relatively low ΔG and K_i values¹⁸.

In SrpA, the test ligands generally form 1–3 H-bonds, with important residues such as Lys340, Lys373, Asp434, Thr372, which are known to be located in the sialic-acid-binding groove of SrpA. When a ligand interacts with these residues, it indicates that the ligand is in the same location as native sialic acid, so the interaction can be said to be overlapping²³. Ligands with lower ΔG (Compound **3** or **4**) also typically show stronger overlap, indicating potential as SrpA-sialoqlycan adhesion inhibitors.

Ligands to FimA show the formation of 2–3 H-bonds with residues such as Lys59, Ser75, Glu70, Val105, which are residues corresponding to the native ligand interaction site (generally in the adhesin groove). When the test ligands bind to these residues, their interactions overlap with the native binding pocket²⁴, indicating that the ligands can block FimA adhesion. Some ligands also interact through hydrophobic contacts (Leu104, Ile73), enhancing the stability of the complex.

Meanwhile, RadD shows a very similar interaction pattern: ligands form 1–3 H-bonds mainly with Gly36, Arg45, Tyr195, Lys73, residues that are part of the RadD interaction domain. Most ligands show overlap with the native ligand binding site, especially if they interact with Arg and Lys, which are the main electrostatic residues in RadD. More negative ΔG values for some ligands indicate the potential of ligands to competitively disrupt the RadD adhesion mechanism²⁵.

In Ddl, ligands form 2–4 hydrogen bonds, mainly with active residues such as Glu223, Asp293, Lys251, Phe295. These residues are located in the catalytic pocket, so the interactions of the test ligands can be categorized as overlapping with the native active site of the ligand (*D*-alanine substrate). Ligands that interact with Glu223 or Lys251 usually have the greatest potential to inhibit the formation of D-Ala-D-Ala, which is critical for cell wall biosynthesis²⁶.



Figure 3. Conformations of the native ligand, *M. oleifera* compounds, and positive controls at SrpA (A), ligand conformational positioning receptor, and (B) Close-up view.

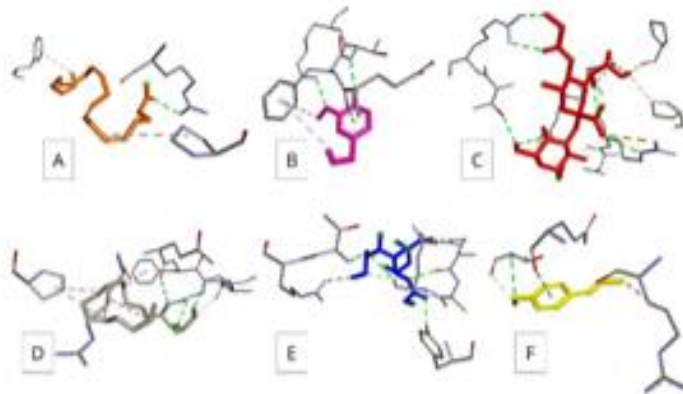


Figure 4. Molecular interactions of SrpA receptor with (A) Arachidonic acid, (B) eugenol, (C) native ligand, (D) phytosphingosine, (E) positive control, and (F) trans-anethole.



Figure 5. Conformations of the native ligand, *M. oleifera* compounds, and positive controls at Cystalytin (A), ligand conformational positioning receptor, and (B) Close-up view.

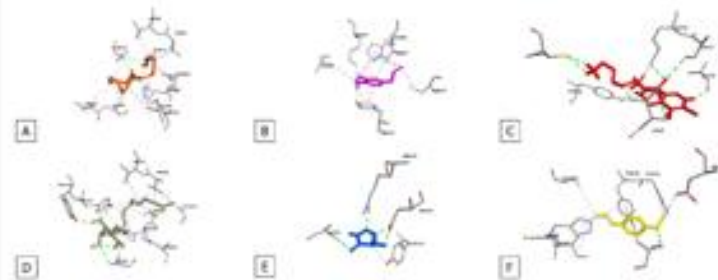


Figure 6. Molecular interactions of Cystalytin receptor with (A) Arachidonic acid, (B) eugenol, (C) native ligand, (D) phytosphingosine, (E) positive control, and (F) trans-Anethole.



Figure 7. Conformations of the native ligand, *M. oliverae* compounds, and positive controls at FimA (A), ligand conformational positioning receptor, and (B) Close-up view.

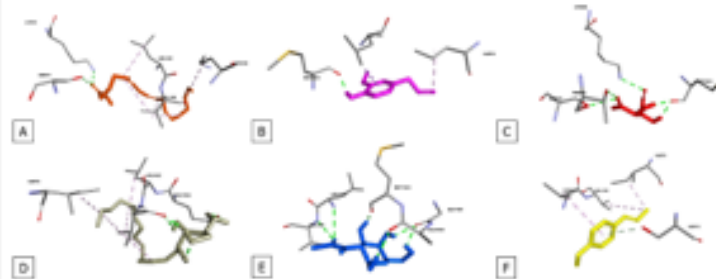


Figure 8. Molecular interactions of FimA receptor with (A) Arachidonic acid, (B) eugenol, (C) native ligand, (D) phytosphingosine, (E) positive control, and (F) trans-anetholes

The complexes of ligand-receptor stabilized their binding in active or binding sites by forming numerous hydrogen bonds across several targets with important catalytic or binding-site residues²⁷. Lower (larger) binding energies and maybe stronger inhibitory effects are the outcome of compounds that can form hydrogen bonds. These compounds are thus more likely to stay anchored inside the active site. For instance, eugenol formed hydrogen bonds with Lys238 and Tyr123 in Cystalytin, important catalytic residues essential for PLP-dependent activity. This deep connection raises the possibility of significant enzyme function disruption. Phytosphingosine presented the most hydrogen bonds compared to the other compounds, which generated an extensive hydrogen bond complex. Hydrogen bond networks are hydrogen bonds that connect the side chains of numerous residues throughout the protein. Hydrogen bond networks stabilize the overall protein structure and have been shown to play a role in activation and allostery²⁸. Eugenol also forms a fairly strong hydrogen bond with the receptor, which is characterized by the number of hydrogen bonds formed. These polar interactions imply that these substances can successfully stabilize their binding to vital virulence proteins, which may interfere with the mechanisms of bacterial colonization or survival²⁹. The conformations of all the ligands were illustrated in **Figures 3, 5, 7, 19, and 11** followed by the molecular interactions of hydrogen bonds and hydrophobic interactions for each ligand in a specific receptor were demonstrated in **Figures 4, 6, 9, 10, and 12**. Each ligand was presented in different color for easier identification of the interactions in those figures, red for native ligand, blue for positive control, orange for arachidonic acid, purple for eugenol, grey for phytosphingosine, and yellow for trans-anethole.

By encouraging van der Waals interactions with nonpolar residues in protein binding sites, hydrophobic interactions play an equally substantial role in ligand affinity in molecular docking. These interactions can be maximized by compounds with long hydrophobic chains or aromatic sections, which improve binding stability and hydrogen bond complementarity^{30, 31}. Phytosphingosine and arachidonic acid showed the most frequent hydrophobic interactions among a number of targets in this analysis, interacting with a wide variety of hydrophobic residues across targets, such as Phe295 and Leu145 in Ddl, Ile73 and Leu105 in FimA, and Ala39 and Ile205 in Cystalytin. For lipophilic compounds, which depend on embedding into hydrophobic pockets to establish effective binding, these interactions are especially significant. The moderate-to-strong binding energies seen for these compounds are explained by the presence of extensive hydrophobic interactions, which in some cases are coupled with hydrogen bonding. This supports the compounds' potential as multi-target inhibitors of oral bacterial virulence factors³².



Figure 10. Conformations of the native ligand, *M. olivera* compounds, and positive controls at RadD (A), ligand conformational positioning receptor, and (B) Close-up view.



Figure 11. Molecular interactions of FimA receptor with (A) Arachidonic acid, (B) eugenol, (C) native ligand, (D) phytosphingosine, (E) positive control, and (F) trans-anethole.



Figure 22. Conformations of the native ligand, *M. olivera* compounds, and positive controls at Ddi (A), ligand conformational positioning receptor, and (B) Close-up view.



Figure 13. Molecular interactions of Ddi receptor with (A) Arachidonic acid, (B) eugenol, (C) native ligand, (D) phytosphingosine, (E) positive control, and (F) trans-anethole.

CONCLUSION

This study found that *Moringa oleifera*-derived compounds—eugenol, trans-anethole, arachidonic acid, and phytosphingosine—exhibit promising multi-target binding affinities against major virulence proteins associated with cariogenic and endodontic infections. Molecular docking demonstrated that phytosphingosine had the most consistent and comprehensive anticipated interactions across various sites, indicating more potential to interfere with multiple bacterial virulence processes at the same time. All ligands tested are capable of interacting directly with the natural binding pockets of Cystalytin, SrpA, FimA, RadD, and Ddi. These interactions consistently involve important catalytic or adhesion-related residues and are supported by the formation of stable hydrogen bonds and multiple hydrophobic contacts. Based on the overall docking profile, these ligands show potential for inhibiting essential enzyme pathways and virulence adhesins. These findings address the research objective by confirming that the compounds studied have multi-target binding capabilities with antibacterial activity through the simultaneous inhibition of pathogen adhesion and metabolic function. The tested compounds could serve as promising lead compounds for the development of multi-target antibacterial agents. Their ability to bind competitively in the native ligand pocket indicates an effective mechanism for inhibiting bacterial virulence factors and essential enzymes, making them relevant candidates for further enzyme evaluation. These results support the concept that molecules derived from natural products can act on multiple bacterial targets, and methodologically demonstrate the usefulness of integrated docking analysis for the initial screening of multi-target inhibitors.

Based on these computational findings, phytosphingosine could be used as a supplementary agent in conservative dental therapy by targeting multiple mechanisms involved in bacterial adhesion, survival, and tissue damage associated with cariogenic and endodontic infections.

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Author Contributions

Conceptualization, MFA, DK, TA, DH; methodology, MFA, DK, TA, DH; software, DK, DH; validation, MFA, DK, TA, DH; formal analysis, MFA, DK, TA, DH; investigation, MFA, DK, TA, DH; resources, MFA, DK, TA, DH; data curation, DK, DH; writing original draft preparation, MFA, DK, TA, DH; writing review and editing, MFA, DK, TA, DH; visualization, DK, DH; supervision, MFA, DK, TA, DH; All authors have read and agreed to the published version of the manuscript.

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Conflicts of Interest: The authors declare no conflict of interest.

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Reviewer ...

The conclusion contains the answers to the research problem formulation, not by including the statistical results, but in the form of conclusions derived.

Meiny F Amin

We appreciate the reviewer's comment. The conclusion section has now been thoroughly revised. The revised conclusion provides a clear synthesis of the findings in direct relation to the stated research objectives.

Reply



Reviewer ...

Please complete it, for an example you can see the previous P/D publication.

Meiny F Amin

Thank you, we have added it.

Reply



Reviewer ...

Please complete it, for an example you can see the previous P/D publication.

Meiny F Amin

Thank you, we have added it.

Reply



Reviewer ...

Please complete it, for an example you can see the previous P/D publication.

Meiny F Amin

Thank you, we have added it.

Reply



Reviewer ...

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**5. Bukti surat manuskrip diterima
30 Maret 2026**



Date: 30 March, 2026

Padjadjaran Journal of Dentistry (PJD)

Manuscript Acceptance Letter

Dears,

Meiny Faudah Amin, Dikdik Kurnia, Taufiq Ariwibowo, Dicky Hardi

We are pleased to inform you that our reviewers have accepted and recommended your manuscript entitled **"Multi-target potential of moringa oleifera-derived compounds against cariogenic and endodontic virulence proteins revealed by molecular docking: An in silico experimental study"** for publication in Vol 38 No 1 of Padjadjaran Journal of Dentistry (PJD).

Thank You for Choosing to Publish in Our Journal

Best Regards

Chief Editor



Prof. Dr. Nina Djustiana, drg, MKes

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Dr Anne Agustina Suwargiani, drg, MKM,

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Multi-target potential of moringa oleifera-derived compounds against cariogenic and endodontic virulence proteins revealed by molecular docking: an in silico experimental study

Meiny Faudah Amin, Dikdik Kurnia, Taufiq Arwibowo, Dicky Hardi

Abstract

Introduction: Dental infections are multifactorial diseases involving bacterial biofilms and host immune responses. Natural compounds with antibacterial activity, such as *Moringa oleifera*, have been explored as alternatives to conventional antibiotics. This study aimed to evaluate the interaction profiles of four *Moringa oleifera*-derived compounds against multiple virulence-associated proteins of cariogenic and endodontic pathogens using in silico molecular docking. **Methods:** This study was an in silico experimental study using molecular docking simulations to evaluate the binding energy of four *M. oleifera*-derived compounds (eugenol, trans-anethole, arachidonic acid, and phytosphingosine) with five key virulence-associated proteins of cariogenic and endodontic pathogens (Cystalytin, SrpA, FimA, RadD, and Ddl) AutoDock 4.0 was used for the docking simulations. Docking results were analyzed based on binding energy (ΔG) and inhibition constant (KI) values. The best binding conformations were selected according to the lowest binding energy and visualized to identify key ligand-protein interactions using Discovery Studio Visualizer. **Results:** The phytosphingosine-Ddl exhibited the lowest binding energy of -7.42 kcal/mol, followed by eugenol with three different receptors (Cystalytin, SrpA, and FimA) and arachidonic acid-RadD. The lowest inhibition constant was shown by the phytosphingosine-Ddl complex at 3.61 μ M. Each compound interacted with various targets, but phytosphingosine exhibited the most consistent and widespread predicted binding via hydrogen bonds with Glu222, Arg291, Glu306, Asp293, Lys251, and hydrophobic interactions of Phe295, Phe245, Phe175, and Leu145. **Conclusion:** This in silico molecular docking study demonstrated that *Moringa oleifera*-derived compounds, particularly phytosphingosine, exhibit strong binding affinity toward key virulence-associated proteins of cariogenic and endodontic pathogens. These findings highlight the potential of *M. oleifera* as a natural source of antibacterial agents and support further experimental validation of its therapeutic applications in oral infections.

Keywords

Molecular docking, moringa oleifera, dental caries, cariogenic bacteria, virulence factors

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ORIGINAL ARTICLE

Multi-target potential of *moringa oleifera*-derived compounds against cariogenic and endodontic virulence proteins revealed by molecular docking: an in silico experimental study

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ABSTRACT

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