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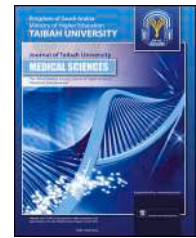
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Brief Communication

In silico evaluation of *Alstonia scholaris* phytochemicals against periodontal pathogens



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المُلخَص

أهداف البحث: تُعدّ البورفيروموناس اللثوية والتريبونيماس السهمية من الجراثيم التابعة لـ المجتمع الأحمر والمترتبة ارتباطاً وثيقاً بمرض اللثة. تعتمد البورفيروموناس اللثوية على مستقبل ارتباط الهيم لاكتساب الهيم، بينما تستخدم التريبونيماس السهمية بروتين الارتباط بعامل الحماية المناعية للتهرب من الاستجابة المناعية. هدفت هذه الدراسة إلى تقييم القدرة التثبيطية لثلاثة مركبات نباتية (الألستونين، إيكيتامين كلوريد، وفيلالالستونين) المستخلصة من نبات الألستونيا ضدّ هذه الأهداف، مع مقارنتها بالمينوكسيسكلين والكلورهيكسدين باستخدام تقنية التحام الجزيئات.

طرق البحث: تم إجراء التحام جزيئي مع التحقق من صحة النتائج عبر إعادة الاختبار، والتأكد من موثوقية المستقبلات (قيمة الانحراف الجذري 1.821 أنغستروم لمستقبل الهيم، و0.851 أنغستروم لمستقبل عامل الحماية). وشملت المقارنة استخدام الكلورهيكسدين والمينوكسيسكلين كضوابط إيجابية. تم تحليل طاقات الارتباط (دلتا جي)، وثوابت التثبيط (كي أي)، وتفاعلات المستقبل مع المركب المرتبط.

النتائج: أظهر مركب إيكيتامين كلوريد أعلى ألفة ارتباط لمستقبل الهيم (دلتا جي -4.86 كيلوسعر/مول؛ ثابت تثبيط 274.96 ميكرومول). بينما كان الألستونين الأكثر ارتباطاً بمستقبل عامل الحماية (دلتا جي -7.44 كيلوسعر/مول؛ ثابت تثبيط 3.53 ميكرومول). وأظهر فيلالالستونين ألفة متوسطة، في حين كان المينوكسيسكلين الأقوى تأثيراً بصورة عامة. وشملت الروابط

الهيدروجينية المحورية الأحماض الأمينية: 178 أرجنين، 70 تربتوفان، و116 تيروزين.

الاستنتاجات: أظهرت المركبات النباتية المستخلصة من الألستونيا، ولا سيما إيكيتامين كلوريد والألستونين، قدرة تثبيطية واعدة، وإن كانت أضعف من المضادات الميكروبية القياسية. وقد تمثل عوامل مساعدة طبيعية محتملة في معالجة أمراض اللثة، مع ضرورة التحقق التجريبي من فعاليتها.

الكلمات المفتاحية: الألستونيا؛ التحام الجزيئات؛ جراثيم اللثة؛ البورفيروموناس اللثوية؛ التريبونيماس السهمية

Abstract

Objectives: *Porphyromonas gingivalis* and *Treponema denticola* are red complex pathogens strongly associated with periodontal disease. *P. gingivalis* relies on the heme-binding receptor HmuY for heme acquisition, whereas *T. denticola* uses factor H-binding protein (FhbB) to evade immune responses. This study was aimed at evaluating the inhibitory potential of three phytochemicals (alstonine, echitamine chloride, and villalstonine) from *Alstonia scholaris* against these targets, which were compared with minocycline and chlorhexidine, via molecular docking.

Methods: Molecular docking was performed with validation by redocking and confirmation of receptor reliability (RMSD 1.821 Å for HmuY and 0.851 Å for FhbB). Chlorhexidine and minocycline were included as positive controls. Binding energies (ΔG), inhibition constants (Ki), and receptor–ligand interactions were analyzed.

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Results: Echitamine chloride exhibited the strongest affinity for HmuY (ΔG -4.86 kcal/mol; K_i 274.96 μM), whereas alstonine bound most strongly to FhbB (ΔG -7.44 kcal/mol; K_i 3.53 μM). Villalstonine showed moderate affinity, whereas minocycline was the most potent overall. Key hydrogen bonds involved ARG178, TRP70, and TYR116.

Conclusions: *A. scholaris* phytochemicals, particularly echitamine chloride and alstonine, displayed promising but weaker inhibitory potential than standard antimicrobials. They therefore might serve as natural adjuncts in periodontal therapy, pending experimental validation.

Keywords: *Alstonia scholaris*; Molecular docking; Periodontal pathogens; *Porphyromonas gingivalis*; *Treponema denticola*

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Introduction

Periodontal disease is a multifactorial condition characterized by polymicrobial dysbiosis, in which key pathogens such as *Porphyromonas gingivalis* and *Treponema denticola* have dominant roles in disease progression. *P. gingivalis* is recognized as a keystone pathogen capable of manipulating the host immune system and reshaping microbial communities to favor dysbiosis. Its survival strongly depends on heme acquisition, as mediated by the heme-binding protein HmuY, which is essential for heme utilization and pathogenic persistence.^{1,2}

Similarly, *T. denticola*, another member of the red complex, markedly contributes to periodontal tissue destruction. It expresses factor H-binding protein B (FhbB), which

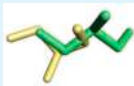
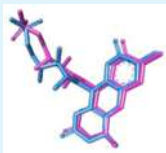
subverts complement regulation by binding host factor H, thereby enabling bacterial survival and immune evasion.^{3,4} The pathogenic synergy between these species exacerbates periodontal breakdown and increases systemic risk.^{5,6} Recent evidence has also demonstrated that the red and orange complex subgingival microbiome is more abundant in older patients with cognitive impairment than in cognitively normal individuals, thereby highlighting a potential link between periodontal pathogens and systemic diseases such as dementia.⁷

Given the growing challenge of antimicrobial resistance, natural compounds are increasingly being investigated as alternative or adjunctive therapeutic agents. Plant-derived bioactive metabolites offer diverse pharmacological activities with relatively low toxicity. *Alstonia scholaris*, a traditional medicinal plant, contains a variety of alkaloids, iridoids, and terpenoids with documented anti-inflammatory, anticancer, and antimicrobial properties.^{8,9} Among its bioactive alkaloids, alstonine, echitamine chloride, and villalstonine are of particular interest. Despite evidence of anticancer and antiparasitic activities, their potential as antibacterial or anti-periodontal agents has not been fully evaluated. In silico molecular docking provides a cost-effective platform to rapidly predict ligand–protein interactions and has become highly relevant in periodontal research.¹⁰ This study was aimed at assessing the binding affinity of selected *A. scholaris* alkaloids toward key virulence factors of *P. gingivalis* (HmuY) and *T. denticola* (FhbB).

Materials and Methods

In silico molecular docking was conducted with the enzyme receptors HmuY from *P. gingivalis* and FhbB from *T. denticola* (PDBID codes 3H8T and 3F2V, respectively). The 3D structures of ligands comprising the investigated compounds and positive controls had CID codes of 441979 (alstonine), 124841315 (echitamine chloride), 5476353

Table 1: Redocking results of the enzyme receptors 3H8T (*P. gingivalis*) and 3F2V (*T. denticola*). Overlay of the native ligand (GOL) between co-crystals (yellow) and redocking (green) of 3H8T receptors, and overlay of the native ligand (FMN) between co-crystals (purple) and redocking (blue) of 3F2V receptors.

Receptor (PDBID)	Native ligand	Residues in disallowed regions (%)	Overlay of the native ligand	RMSD (Å)	Active site coordinates (x:y:z)
3H8T	GOL	0.6		1.821	-25.345: 24.372: 23.615
3F2V	FMN	0		0.851	14.067: -7.693: 23.334

GOL: Glycerol; FMN: Flavin mononucleotide; Å: Ångström.

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Table 2: Docking results of compounds with the 3H8T (*P. gingivalis*) and 3F2V (*T. denticola*) enzyme receptors.

No.	compounds	3H8T (<i>P. gingivalis</i>)				3F2V (<i>T. denticola</i>)					
		ΔG (kcal/mol)	Hydrogen interaction	Hydrophobic interaction	Ki (μM)	3D interaction	ΔG (kcal/mol)	Hydrogen interaction	Hydrophobic interaction	Ki (μM)	3D interaction
1.	Alstonine	-4.77	ARG178 and SER176	THR102 and LYS101	317.80		-7.44	TRP70; GLY110; and TYR116	TYR69 and PRO67	3.53	
2.	Echitamine chloride	-4.86	GLU103; LYS101; THR102; and GLY100	—	274.96		-7.39	TRP70 and TYR116	—	3.86	
3.	Villalstonine	-4.81	LYS101; THR102; GLN106; and GLU103	—	296.39		-4.97	—	PHE71	225.75	
4.	Minocycline	-5.10	LYS101; THR102; GLY100; and GLU103	—	182.84		-7.86	LEU109; GLY110; TYR116; and PHE71	TYR69 and TRP70	1.74	
5.	Chlorhexidine	-5.27	SER176; THR102; and GLU103	ARG178 and LYS177	136.84		-7.18	ILE68; GLY110; and TYR116	HIS10; PRO67; HIS19; ALA11; TYR69; PHE71; and TRP70	5.42	

ΔG : Binding affinity; Ki: inhibition constant; ALA: Alanine; ARG: Arginine; GLN: Glutamine; GLU: Glutamic acid; GLY: Glycine; HIS: Histidine; LYS: Lysine. PHE: Phenylalanine; PRO: Proline; SER: Serine; THR: Threonine; TRP: Tryptophan; TYR: Tyrosine.

(villalstonine), 9552079 (chlorhexidine), and 54675783 (minocycline). Chlorhexidine and minocycline served as positive controls for validating the docking protocol and were selected because of their established antimicrobial activity against oral pathogens. The computational methods were performed on an Asus Vivobook 14 laptop with an Intel(R) Pentium(R) CPU 5405U 2.30 GHz processor, 8.00 GB RAM, and a 64-bit operating system (x64-based processor). The software included BIOVIA Discovery Studio v24.1.0.23298 (San Diego, California, USA), AutoDock 4 Version 1.5.7 (La Jolla, California, USA), and ChemDraw 3D Version 3.0 (CambridgeSoft/PerkinElmer; headquartered in Waltham, Massachusetts, USA).

We determined receptor conformation by downloading the receptor structure from [RCSB.org](https://www.rcsb.org). The conformational suitability of the receptor was tested on the [saves.org](https://www.saves.org) web server with Ramachandran plot calculations. Redocking was conducted by separating the native ligand from the receptor in BIOVIA Discovery Studio software. The native ligand and receptor were docked in AutoDock 4 with the grid box centered on the ligand coordinates. Running redocking involved 100 runs with the genetic algorithm. The redocking results were visualized in BIOVIA Discovery Studio (San Diego, California, USA). Docking of compounds and positive controls (ligands) with the 3H8T and 3F2V receptors was performed on the active site coordinates obtained from the redocking results. Ligand energy was minimized in ChemDraw 3D (CambridgeSoft/PerkinElmer; headquartered in Waltham, Massachusetts, USA) with the MM2 method. The ligand and receptor were docked with AutoDock 4.7 (La Jolla, California, USA) and visualized in BIOVIA Discovery Studio (San Diego, California, USA).

Results

In the Ramachandran plot test, the receptor conformation was indicated by <2 % of residue values in disallowed regions. The values of residues in disallowed regions for the 3H8T and 3F2V receptors were 0.6 % and 0 %, respectively. The RMSD value subsequently corroborated the outcomes of the Ramachandran plot assessment. The RMSD values for the 3H8T and 3F2V receptors were 1.821 Å and 0.851 Å. Beyond the RMSD values, redocking indicated the active site coordinates of the receptors. The active site coordinates (x:y:z) of the *P. gingivalis* and *T. denticola* receptors were -25.345: 24.372: 23.615, and 14.067: -7.693: 23.334, respectively (Table 1).

Data for docking of alstonine, echitamine chloride, villalstonine, and the positive controls with the 3H8T and 3F2V receptors are presented in Table 2. Among the three active chemicals of *A. scholaris*, echitamine chloride exhibited the highest binding affinity to the 3H8T receptor (-4.86 kcal/mol) yet remained inferior to the positive controls minocycline and chlorhexidine (-5.10 and -5.27 kcal/mol, respectively). In contrast to the 3F2V receptor findings, the binding affinity of alstonine and echitamine chloride (-7.44 and -7.39 kcal/mol) exceeded that of chlorhexidine (-7.18 kcal/mol).

Discussion

The crystallographic structures in this study contained multiple ligands that required careful consideration for docking validation. In the 3H8T structure of *P. gingivalis* HmuY, three ligands were present: heme, glycerol (GOL), and sulfate (SO₄). For methodological consistency, GOL served as the reference ligand in redocking validation, because it was resolved with clear coordinates in the deposited structure, thus enabling RMSD calculation. Similarly, in the 3F2V structure of *T. denticola* FhbB, flavin mononucleotide was resolved as a co-crystallized ligand. Because it was included to stabilize the structure during crystallization, it served as the native ligand for redocking. Use of these deposited ligands (GOL for 3H8T and flavin mononucleotide for 3F2V) enabled reliable validation of docking accuracy via RMSD values, thus providing confidence in the subsequent docking analysis of *A. scholaris* phytochemicals.

Validation of the receptor conformation showed acceptable geometry, with <2 % of residues in disallowed regions for both HmuY (3H8T) and FhbB (3F2V). RMSD values of 1.821 Å and 0.851 Å confirmed the reliability of the docking protocol, because values below 2.5 Å indicate consistent redocking accuracy. A detailed analysis of docking interactions revealed that several residues contributed to the stability of ligand binding. In the HmuY receptor, TRP70, TYR116, and LYS101 were key residues mediating hydrogen bonding and hydrophobic interactions that stabilized the ligand-receptor complex. Echitamine chloride formed hydrogen bonds with LYS101 and THR102, whereas TRP70 and TYR116 contributed to π - π stacking and hydrophobic stabilization, thereby producing a conformation similar to that of the positive controls. These interactions suggested that the phytochemicals mimic the binding orientation of native ligands within the heme pocket and might potentially interfere with the heme acquisition essential for *P. gingivalis* survival. This pattern was consistent with previous *in silico* reports identifying aromatic residues such as TRP and TYR to be critical for ligand anchoring in *P. gingivalis* heme-binding domains.⁹⁻¹¹

Docking analysis (Table 2) revealed that echitamine chloride demonstrated the strongest binding affinity to *P. gingivalis* HmuY ($\Delta G = -4.86$ kcal/mol), which was similar to the binding affinities of the positive controls chlorhexidine (-5.27 kcal/mol) and minocycline (-5.10 kcal/mol). This compound also shared multiple hydrogen bond interactions with key residues (LYS101, THR102, and GLY100), similarly to the positive controls, thus supporting its potential as an HmuY inhibitor. Whereas villalstonine showed moderate binding affinity ($\Delta G = -4.81$ kcal/mol), alstonine exhibited slightly weaker binding ($\Delta G = -4.77$ kcal/mol). Nevertheless, villalstonine was assessed in this study because it is a principal alkaloid of *A. scholaris*, and it provided valuable comparative insight into how subtle structural differences among related compounds influence receptor binding. The finding that villalstonine binding relies primarily on hydrophobic interactions is supported by previous reports suggesting that

both polarity and conformational flexibility are critical for optimal ligand accommodation in heme-binding proteins.^{1,2,9}

Interestingly, alstonine and echitamine chloride, compared with chlorhexidine, displayed superior binding affinity toward *T. denticola* FhbB (3F2V) (−7.44, −7.39, and −7.18 kcal/mol, respectively). Minocycline remained the most potent ligand (−7.86 kcal/mol). These findings suggested that *A. scholaris* alkaloids, particularly alstonine, might be more effective against *T. denticola* than conventional agents. The inhibition constants also corroborated this finding: alstonine and echitamine chloride showed low micromolar values (3.5–3.8 μM) approaching those of minocycline (1.74 μM).

These results aligned with findings from previous reports highlighting the promise of natural compounds in disrupting bacterial virulence mechanisms and modulating biofilm formation.^{8,11} *A. scholaris* alkaloids have shown antimicrobial and anti-inflammatory potential, thus suggesting their pharmacological promise.^{10,12} The residue-level interactions observed herein support their potential as adjunctive natural agents in periodontal therapy by disrupting bacterial heme uptake and complement evasion mechanisms. This study's strengths include its focused targeting of key virulence factors and validated docking accuracy with acceptable RMSD values. The comparative analysis with standard antimicrobials added translational relevance. However, because of its in silico design, this study cannot fully replicate biological conditions such as compound stability and in vivo pharmacodynamics.

Conclusion

Among the evaluated *A. scholaris* phytochemicals, echitamine chloride demonstrated the highest potential in inhibiting the HmuY receptor of *P. gingivalis*, whereas alstonine showed superior binding to the FhbB receptor of *T. denticola*. These findings highlight the therapeutic promise of *A. scholaris*-derived compounds as adjunctive agents for periodontitis. Further in vitro and in vivo validation is necessary to confirm their antimicrobial efficacy, bioavailability, and safety profiles. Such studies will be essential to establish the translational potential of *A. scholaris* compounds as plant-based adjuncts in evidence-based periodontal care.

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Conflict of interest

The authors declare no relevant conflicts of interest related to this study.

Ethical approval

This study did not involve human participants, animals, or identifiable personal data. Therefore, ethical approval was

not required, and there are no ethical issues associated with the conduct of this research.

Author contributions

MIR conceived and designed the study; contributed to data acquisition, analysis, and interpretation; and was a major contributor in drafting and revising the manuscript. SH participated in data acquisition, analysis, and drafting of the manuscript, and contributed to its critical revision. MOR was involved in data analysis and interpretation, as well as revision of the manuscript for important intellectual content. KK, CTB, and AC contributed to the critical review and intellectual revision of the manuscript. All authors have critically reviewed and approved the final draft and are responsible for the content and similarity index of the manuscript.

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