Volume 21 Issue 1 February 2026

ELSEVIER

Journal of Taibah University Medical Sciences

Indexed with
Scopus, Web of Science, PubMed Central, and
Directory of Access Journals (DOAJ)
A full member of Committee on Public Ethics (COPE).

ISSN: 1658-3612

Journal of Taibah University Medical Sciences

Open access

3.5 CiteScore | 1.9 Impact Factor

Volume 21, Issue 1

Pages 1-190 (February 2026)

Allied health sciences

Pharmacy

Pages 67-77

View PDF Article preview

Clinical Medicine

Review article *Open access*

Shaping the future of surgery: A scoping review of current robotic practices in KSA

Abdulaziz M. Saleem, Mohammed F. Alhazmi, Moaz W. Abulfaraj, Ahmed S. Aljeraisi, Murad M. Aljiffry

Pages 1-14

View PDF Article preview

Research article *Open access*

Pain determinants during office hysteroscopy: Insights from clinical and procedural factors: A nine-year prospective cohort study

Wassan Nori, Zeena R. Helmi, Rafal M. Murshid

Pages 104-113

View PDF

Correspondence *Open access*

Reframing the one health approach to antimicrobial resistance: The epidemiologic significance of environmental water quality

Christian Joseph N. Ong, Jerico B. Ogaya, Rahmatullah Nazari, Mohamed M. Ahmed, Don E. Lucero-Prisno

Pages 114-115

View PDF

Case report *Open access*

Effects of a pulmonary rehabilitation program in a patient with very severe chronic obstructive pulmonary disease at a primary care center: A case report

Mohammed E. Alsubaiei

Pages 129-134

View PDF

Case report *Open access*

New-onset atrial fibrillation in a healthy young adult following electronic cigarette use

Talal Alzahrani

Pages 135-138

View PDF Article preview

Research article *Open access*

Exploratory analysis of immune profiles in 2- to 3-year-old children with growth stunting

Rizana Fajrunni'mah, Mohamad Sadikin, Heri Wibowo, Dwirini Retno Gunarti

Pages 139-148

View PDF Article preview

Case report *Open access*

Bronchiectasis in a child with a homozygous *DCDC2* gene mutation: A case report

Khulud S. AlSaedi, Ahlam A. Mazi

Pages 159-163

View PDF Article preview

Dentistry

Short communication *Open access*

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

Muhammad I. Rizal, Syafia Husain, Komariah Komariah, Ciptadhi T. Binartha, ... Moehamad O. Roeslan

Pages 25-30

View PDF Article preview

Research article *Open access*

Effects of gold nanoparticles and apricot seeds on bone healing in New Zealand rabbits

Zena J. Wally, Bushra H. Al-Maula, Sahar G. AL-Kazzaz, Rasha H. Dosh, ... Julfikar Haider

Pages 78-90

View PDF Article preview

Research article *Open access*

Acupressure versus paracetamol for short-term orthodontic pain: A randomized clinical trial

Yassir A. Yassir, Ayat M. Hussein, Rawof R. Al Tuma

Pages 116-128

View PDF Article preview

Research article *Open access*

Biological evaluation of resin-modified glass ionomer cement containing coumarin derivatives for dental application

Fatimah S.A. Rahman, Dasmawati Mohamad, Nor A.F. Azlisham, Hasnah Osman

Pages 149-158

View PDF Article preview

Health professions education

Correspondence *Open access*

Reframing AI chatbots as cultural and educational catalysts in health professions education

Riza Amalia

Pages 31-32

View PDF

Research article *Open access*

Use of ChatGPT in physical therapy education: Comparative study of usefulness to students and ease of use perceptions, and descriptions of usage patterns

Salwa B. El-Sobkey, Mahmoud ElKholy, Mariam Abdallah, Dina Al-Amir Mohamed, Tayseer Abdeldayem

Pages 178-189

View PDF Article preview

Multidisciplinary research

Review article *Open access*

From diagnostics to education: Multi-domain evaluation of LLM chatbots in neurology

Gopi Battineni, Nalini Chintalapudi, Venkata R. Dhulipalla, Francesco Amenta

Pages 15-24

View PDF Article preview

Research article *Open access*

Lunar synchronization of hemostasis and immunity validates prophetic timing of hijama therapy: A multicenter study from Yemen

Naif T. Ali, Radfan S. Abdullah, Ibrahim Ahmed, Othman Mohammed, ... Abdulmajeed Abdualkareem

Pages 33-40

View PDF

Research article *Open access*

Association between elevated PRIM1 expression and poor prognosis in human urothelial carcinoma

Ban A. Al-Hassany, Israa M. Al-Sudani

Pages 41-48

View PDF Article preview

Research article *Open access*

Mesenchymal and neural stem cell differentiation into Purkinje-like cells: Morphological study

Maeda H. Mohammad, Ahmed M. Al-Shammari, Ahmad A. Aljuboori, Rafal Hussamildeen, Zaid A. Al-Hilli

Pages 164-177

View PDF Article preview

Previous vol/issue Next vol/issue

About this publication

ISSN: 1658-3612

Journal of Taibah University Medical Sciences
Open access

Editorial board

Editorial board by country/region

24 editors and editorial board members in 7 countries/regions

1 Saudi Arabia (17)

2 United Kingdom (2)

3 Canada (1)

See more editors by country/region

Editor-in-Chief

Professor Abdulmohsen Hamdan Al-Zalabani, MD, ABCM, MHPE

Taibah University, College of Medicine, Department of Family and Community Medicine, Al Madinah Al Munawwarah, Saudi Arabia

Epidemiology, Preventive Medicine

Deputy Editors-in-Chief

Assoc. Professor Anwar Abdulfattah A Sayed, MSc, MPH, PhD

Taibah University, College of Medicine, Department of Basic Medical Sciences, Madinah, Saudi Arabia

Medical Microbiology and Immunology, Public Health, Infectious Diseases, Medical Education

Assoc. Professor Walaa Abdullah Mumena, PhD

Taibah University, Faculty of Applied Medical Sciences, Department of Clinical Nutrition, Madinah, Saudi Arabia

Human Nutrition, Nutritional Epidemiology

Journal of Taibah University Medical Sciences

Journal of Taibah University Medical Sciences

Assistant Editors

Editorial Board

Journal of Taibah University Medical Sciences

Submit your article

Journal of Taibah University Medical Sciences

Netherlands | Universities and research institutions | Media Ranking

Country
Netherlands

Subject Area and Category
Medicine
Medicine (miscellaneous)

Publisher
Elsevier B.V.

SCIMAGO INSTITUTIONS RANKINGS

SCImago Media Rankings

SJR 2024
0.480

Q3

H-Index
37

Publication type
Journals

ISSN
16583612

Coverage
2009-2025

Information
Home
How to publish in this journal
Contact

Scope
The Journal of Taibah University Medical Sciences is a bi-monthly peer reviewed publication. Authors are invited to submit articles for publication, reporting original work in clinical and basic medical sciences covering topics from Medicine, Dentistry, Nursing, Pharmacy, and Applied Medical Sciences. Review and Editorial articles are by invitation only. However, those received and found to be of an outstanding nature will be considered for publication. Other regular features within the journal include, Case Reports, Letters to the Editor, and Updates which detail symposia, conferences and workshops located primarily in the Kingdom of Saudi Arabia and the Gulf countries. The

Journal has recently devoted a new Students' Section where the research projects written by the students shall be entertained. All students from the medical, dental, and allied science faculties are invited to participate in this educational and research activity. The peer review shall be performed by senior academicians with a view to guide and supervise the students in medical research and publications.

Quartiles

Medicine (miscellaneous)	2017	Q3
Medicine (miscellaneous)	2018	Q3
Medicine (miscellaneous)	2019	Q3
Medicine (miscellaneous)	2020	Q3
Medicine (miscellaneous)	2021	Q3
Medicine (miscellaneous)	2022	Q3
Medicine (miscellaneous)	2023	Q3
Medicine (miscellaneous)	2024	Q3

Find similar journals

All quartiles All countries All subject categories Clear filters Download

Only Open Access Journals

1 - Malaysian Journal of Medicine and Health Sciences

62%

similarity

2 - Open Access Macedonian Journal of Medical Sciences

61%

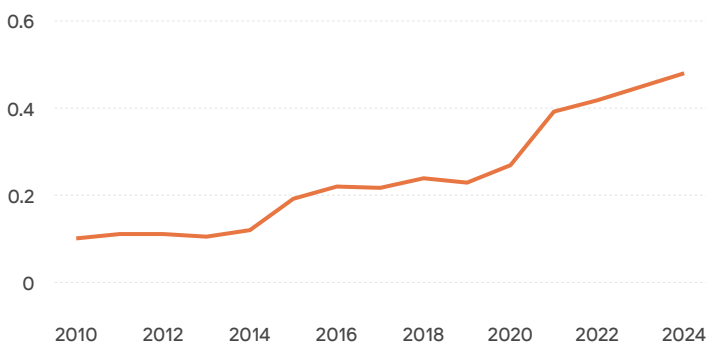
similarity

3 - Health Science Reports

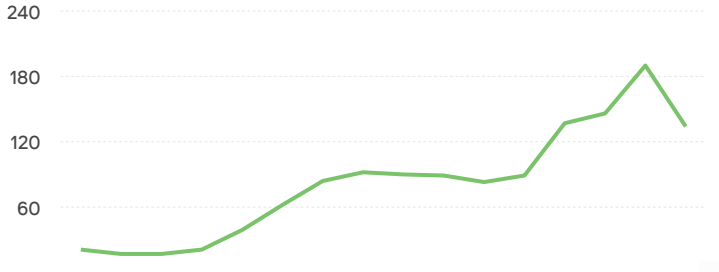
59%

similarity

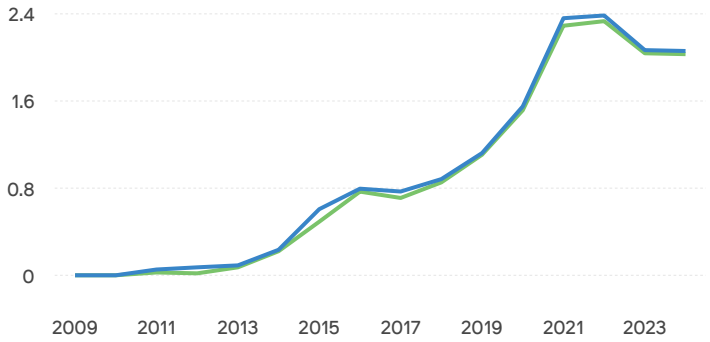
SJR



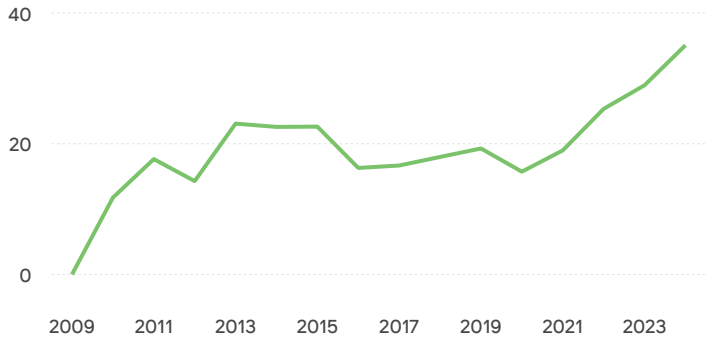
Total Documents



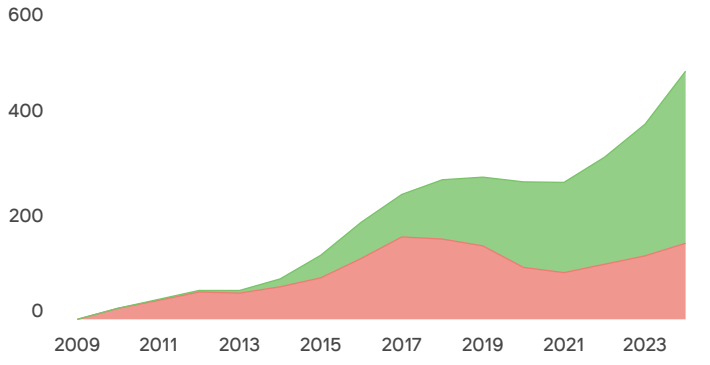
External Cites per Doc Cites per Doc



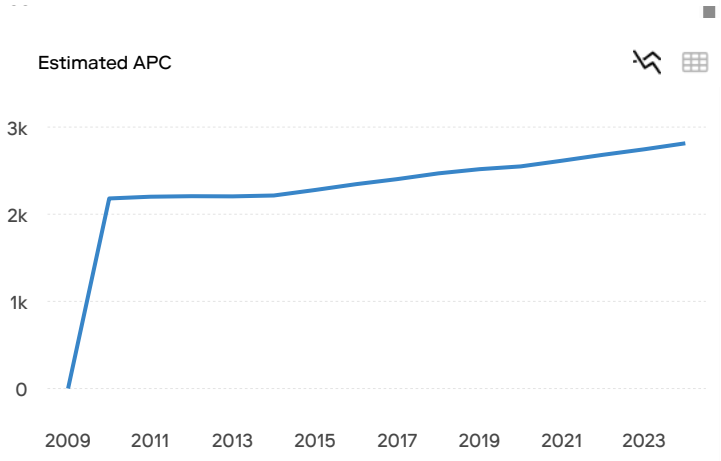
% International Collaboration

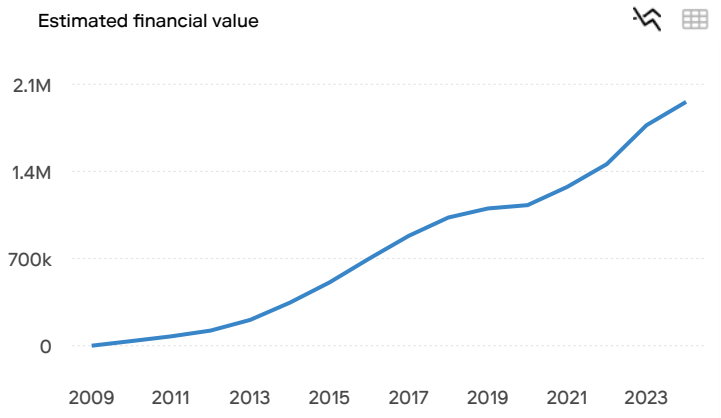


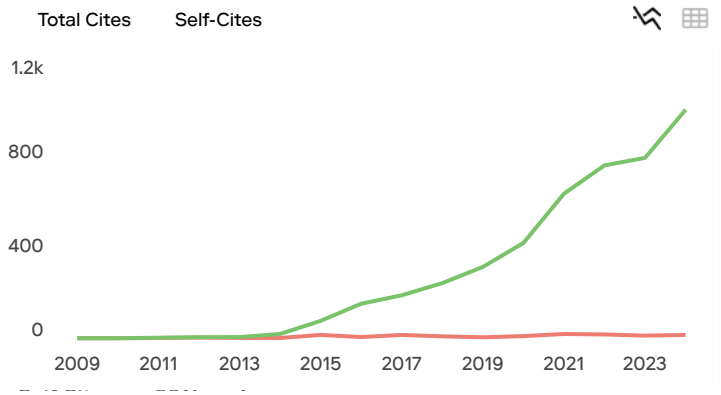
Cited documents Uncited documents



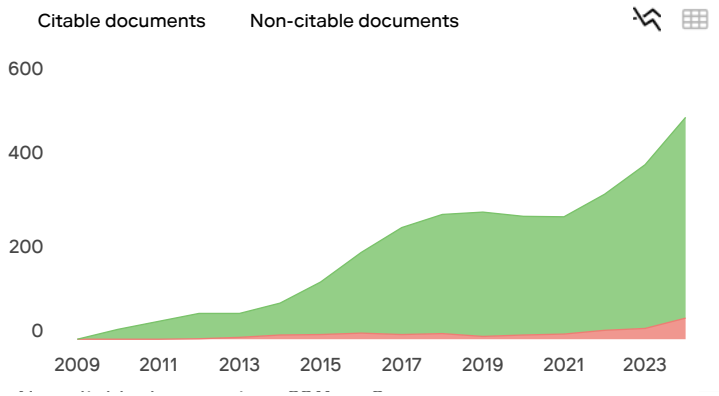
% Female Authors

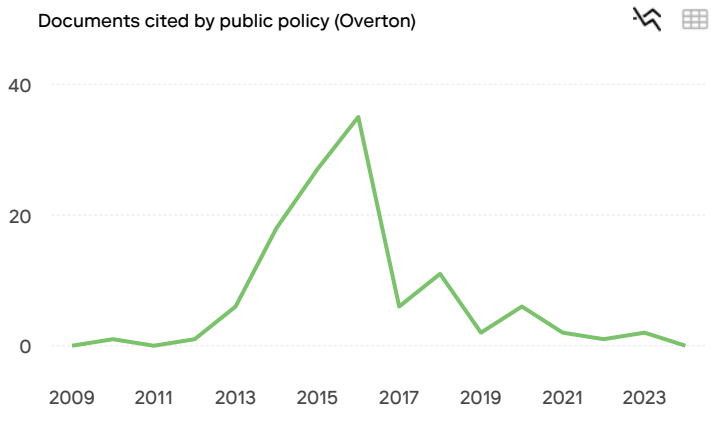


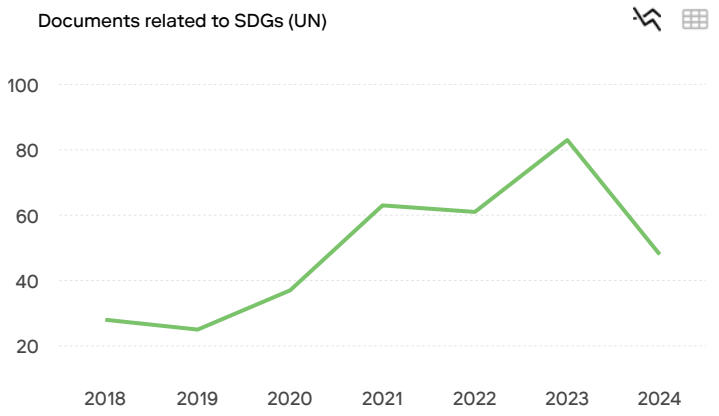




Citations per document







← Show this widget in your own website

Just copy the code below and paste within your html code:

```
<a href="https://www.scimago
```

islamy rahma
1 year ago

I verified the Scopus index and found that it is in quartile 1, with a 75% score. However, the SJR is still in Q3, not Q1.

reply

Melanie Ortiz
1 year ago

Dear Islamy,
Thank you for contacting us.
As you probably already know, our data come from Scopus, they annually send us an update of the data. This update is sent to us around April / May every year.
The calculation of the indicators is performed with the copy of the Scopus database provided to us annually. Regarding your inquiry about the Quartile distribution process at SCImago, the journals are ranked and distributed in 4 equal groups based on their SJR value, unlike Scopus, who ranks the publications by percentiles based on the journal's CiteScore.
The Quartile methodology, like others that are used to group results such as percentiles, can be applied to any indicator. Currently, Scopus offers information on the journals ranking and the percentile they occupy according to the CiteScore indicator (https://service.elsevier.com/app/answers/detail/a_id/14880/supporthub/scopus/), which is perceived as an impact indicator, but that is different from the SJR, as the latter is also a normalized impact indicator (https://www.scimagojr.com/files/SJR2.pdf).
Both Scopus and SCImago Journal and Country Rank offer information on the SJR indicator for every journal, although the position of each of the publications and the quartile in which it is located according to the SJR can be consulted at https://www.scimagojr.com.
According to the above, the difference in the information consulted on the Scopus journal's profile and in Scimagojr.com lies in the fact that they represent the position of the journal based on two different indicators, which are not directly comparable because they measure two different dimensions: Impact (CiteScore) and Normalized Impact (SJR).
Additionally, it is important to keep in mind that, although the quartiles in SJR tend to be distributed in 4 groups of equal size and that the journals appear sorted by the highest SJR to the lowest SJR, it is not always possible due to ties in SJR values and, therefore, journals with the same SJR must be distributed

within the same quartile, which may lead to differences in the number of journals within that quartile.
Best Regards,
SCImago Team

C **Citrawati Wungu**
3 years ago

The process of review in this journal is so slow. It is hard for them to find any reviewers. My manuscript was rejected after they had contacted 26 or more reviewers and no one agreed to review

reply

Melanie Ortiz
3 years ago

Dear Citrawati, thanks for your participation! Best Regards, SCImago Team

T **Triyana Puspa Dewi**
3 years ago

Dear schimago admin,
i would like to ask, is this journal coverage by scopus?

reply

Melanie Ortiz
3 years ago

Dear Triyana, thank you very much for your comment. We suggest you consult the Scopus database directly. Keep in mind that the SJR is a static image (the update is made one time per year) of a database (Scopus) which is changing every day.
The Scopus' update list can also be consulted here:
https://www.elsevier.com/solutions/scopus/how-scopus-works/content
Best Regards, SCImago Team

M **Maram Ahmed**
5 years ago

Hi

I would like to know if this journal is an ISI journal or not?

reply

Melanie Ortiz
5 years ago

Dear Maram,
Thank you for contacting us.
SJR is a portal with scientometric indicators of journals indexed in Elsevier/Scopus. Unfortunately, we cannot help you with your request referring to the index status. We suggest you consult Scopus database (see the current status of the journal) or the mentioned database for further information.
Best Regards, SCImago Team

F **Fatimah**
5 years ago

Hello,

I just wanted to ask, will research in medical engineering applications be acceptable in the journal?

Thank you.

reply

Melanie Ortiz
5 years ago

Dear Fatimah,
thank you for contacting us.
Unfortunately, we cannot help you with your request, we suggest you visit the journal's homepage (See scope and submission/author guidelines) or contact the journal's editorial staff , so they could inform you more deeply.
Best Regards, SCImago Team

Name

Email

Message

I'm not a robot

reCAPTCHA
Privacy - Terms

Send

The users of Scimago Journal & Country Rank have the possibility to dialogue through comments linked to a specific journal. The purpose is to have a forum in which general doubts about the processes of publication in the journal, experiences and other issues derived from the publication of papers are resolved. For topics on particular articles, maintain the dialogue through the usual channels with your editor.

Journal of Taibah University Medical Sciences (2026) 21(1), 25–30

Taibah University

Journal of Taibah University Medical Sciences

www.sciencedirect.com

Brief Communication

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

Muhammad I. Rizal, PhD [a,b], Syafia Husain, BDS [b], Komariah Komariah, PhD [a], Ciptadhi T. Binartha, PhD [a], Arief Cahyanto, PhD [c,d] and Moehamad O. Roeslan, PhD [a,*]

[a] *Department of Oral Biology, Faculty of Dentistry, Universitas Trisakti, Jakarta, Indonesia*
[b] *Center of Molecular Biology Study, Faculty of Dentistry, Universitas Trisakti, Jakarta, Indonesia*
[c] *Department of Clinical Sciences, College of Dentistry, Ajman University, Ajman, United Arab Emirates*
[d] *Centre of Medical and Bio-allied Health Sciences Research, Ajman University, Ajman, United Arab Emirates*

Received 2 September 2025; revised 4 November 2025; accepted 12 December 2025

الملخّص

أهداف البحث: تُعَدّ البورفيروموناس اللثوية والتريبونيما السهمية من الجراثيم التابعة لـ المجمّع الأحمر والمرتبطة ارتباطًا وثيقًا بمرض اللثة. تعتمد البورفيروموناس اللثوية على مستقبل ارتباط الهيم لاكتساب الهيم، بينما تستخدم التريبونيما السهمية بروتين الارتباط بعامل الحماية المناعية للتهرب من الاستجابة المناعية. هدفت هذه الدراسة إلى تقييم القدرة التثبيطية لثلاثة مركّبات نباتية (الألستونين، إيكيتامين كلوريد، وفيلاألستونين) المستخلصة من نبات الألستونيا ضدّ هذه الأهداف، مع مقارنتها بالمينوكسيسكلين والكلورهيكسيدين 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 الكلورهيكسيدين والمينوكسيسكلين كضوابط إيجابية. تم تحليل طاقات الارتباط (دلتا جي)، وثوابت التثبيط (كي آي)، وتفاعلات المستقبل مع المركّب المرتبط.

النتائج: أظهر مركّب إيكيتامين كلوريد أعلى ألفة ارتباط لمستقبل الهيم (دلتا جي −4.86 كيلوسعر/مول؛ ثابت تثبيط 274.96 ميكرومول). بينما كان الألستونين الأكثر ارتباطًا بمستقبل عامل الحماية (دلتا جي −7.44 كيلوسعر/مول؛ ثابت تثبيط 3.53 ميكرومول). وأظهر فيلاألستونين ألفة متوسطة، في حين كان المينوكسيسكلين الأقوى تأثيرًا بصورة عامة. وشملت الروابط الهيدروجينية المحورية الأحماض الأمينية: 178 أرجنين، 70 تربتوفان، و116 تيروزين.

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

الكلمات المفتاحية: الألستونيا؛ التحام الجزيئات؛ جراثيم اللثة؛ البورفيروموناس اللثوية؛ التريبونيما 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 phytocompounds (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.

* Corresponding address: Jalan Kyai Tapa no. 260 Grogol, Jakarta Barat, Jakarta, 11440, Indonesia.
E-mails: ihsan.rizal@trisakti.ac.id (M.I. Rizal), orliando.roeslan@trisakti.ac.id (M.O. Roeslan)

Peer review under responsibility of Taibah University.

Production and hosting by Elsevier

 https://doi.org/10.1016/j.jtumed.2025.12.006

Results: Echitamine chloride exhibited the strongest affinity for HmuY (ΔG −4.86 kcal/mol; Ki 274.96 μM), whereas alstonine bound most strongly to FhbB (ΔG −7.44 kcal/mol; Ki 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*

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]

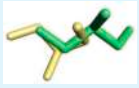
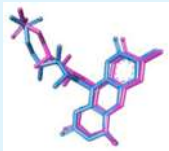
Similarly, *T. denticola*, another member of the red complex, markedly contributes to periodontal tissue destruction. It expresses factor H-binding protein B (FhbB), which subverts complement regulation by binding host factor H, thereby enabling bacterial survival and immune evasion.[3,4] The pathogenic 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

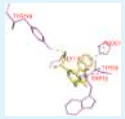
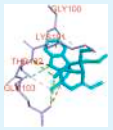
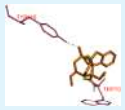
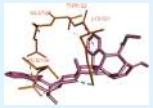
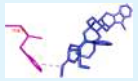
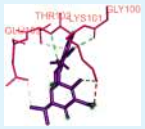
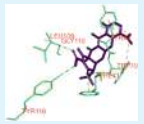
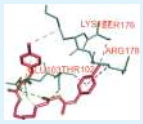
In silico molecular docking was conducted with the enzyme receptors HmuY from *P. gingivalis* and FhbB from *T. denticola* (PDBID codes 3H8T and 3F2V, respectively). The 3D structures of ligands comprising the investigated compounds and positive controls had CID codes of 441979 (alstonine), 124841315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

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

No.	compounds	3H8T (*P. gingivalis*)					3F2V (*T. denticola*)				
		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. The conformational suitability of the receptor was tested on the 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 (SO_4). 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 (ΔG = −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 (ΔG = −4.81 kcal/mol), alstonine exhibited slightly weaker binding (ΔG = −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.

Source of funding

This research was supported by Universitas Trisakti under an internal grant (No. 1033/PUF/FKG/2024−2025).

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.

Acknowledgments

The authors express gratitude to Rizal Padilah for assistance in the computer laboratory.

References

1. Chopra A, Bhat SG, Sivaraman K. *Porphyromonas gingivalis* adopts intricate and unique molecular mechanisms to survive and persist within the host: a critical update. **J Oral Microbiol 2020**; 12(1): 1801090. https://doi.org/10.1080/20002297.2020.1801090.
2. Carvalho-Filho PC, Gomes-Filho IS, Meyer R, Olczak T, Xavier MT, Trindade SC. Role of *Porphyromonas gingivalis* HmuY in immunopathogenesis of chronic periodontitis. **Mediat Inflamm 2016**; 2016: 7465852. https://doi.org/10.1155/2016/7465852.
3. Miller DP, Oliver LD Jr, Tegels BK, Reed LA, O'Bier NS, Kurniyati K, et al. The *Treponema denticola* FhbB protein is a dominant early antigen that elicits FhbB variant-specific antibodies that block factor h binding and cleavage by dentilisin. **Infect Immun 2016**; 84(7): 2051−2058. https://doi.org/10.1128/iai.01542-15. 23.
4. Miller DP, Bell JK, McDowell JV, Conrad DH, Burgner JW, Héroux A, et al. Structure of factor H-binding protein B (FhbB) of the periopathogen *Treponema denticola*: insights into progression of periodontal disease. **J Biol Chem 2012**; 287(16): 12715−12722. https://doi.org/10.1074/jbc.M112.339721.
5. Lamont RJ, Koo H, Hajishengallis G. The oral microbiota: dynamic communities and host interactions. **Nat Rev Microbiol 2018**; 16(12): 745−759. https://doi.org/10.1038/s41579-018-0089-x.
6. How KY, Song KP, Chan KG. *Porphyromonas gingivalis*: an overview of periodontopathic pathogen below the gum line. **Front Microbiol 2016**; 7: 53. https://doi.org/10.3389/fmicb.2016.00053.
7. Tadjoedin FM, Masulili SLC, Rizal MI, Kusdhany LS, Turana Y, Ismail RI, Bachtiar BM. The red and orange complex subgingival microbiome of cognitive impairment and cognitively normal elderly with periodontitis. **Geriatrics 2022**; 7(1): 12. https://doi.org/10.3390/geriatrics7010012.
8. Pasupuleti MK, Nagate RR, Alqahtani SM, Penmetsa GS, Gottumukkala SNVS, Ramesh KSV. Role of medicinal herbs in periodontal therapy: a systematic review. **J Int Soc Prev Community Dent 2023**; 13(1): 9−16. https://doi.org/10.4103/jispcd.JISPCD_210_22. 27.

9. Chhajed M, Jain A, Pagariya A, Dwivedi S, Jain N, Taile V. *Alstonia scholaris* Linn. R. Br.: an assessment of its botany, conventional utilization, phytochemistry, and pharmacology. **Pharm Rev 2023**; 17(33): 184–203. https://doi.org/10.5530/097627870302.
10. Zhao Q, Wang K, Hou L, Guo L, Liu X. Based on network pharmacology and molecular docking to explore the potential mechanism of shikonin in periodontitis. **BMC Oral Health 2024**; 24(1). https://doi.org/10.1186/s12903-024-04618-7. 24.
11. Mishra R, Panda AK, De Mandal S, Shakeel M, Bisht SS, Khan J. Natural anti-biofilm agents: strategies to control biofilm-forming pathogens. **Front Microbiol 2020**; 11: 566325. https://doi.org/10.3389/fmicb.2020.566325.
12. Roeslan MO, Dechatiwongse Na Ayudhya T, Yingyongnarongkul B-E, Koontongkaew S. Anti-biofilm, nitric oxide inhibition and wound healing potential of purpurin-18 phytyl ester isolated from *Clinacanthus nutans* leaves. **Biomed Pharmacother 2019**; 113: 108724. https://doi.org/10.1016/j.biopha.2019.108724.

How to cite this article: Rizal MI, Husain S, Komariah K, Binartha CT, Cahyanto A, Roeslan MO. In silico evaluation of *Alstonia scholaris* phytochemicals against periodontal pathogens. J Taibah Univ Med Sc 2026;21(1):25–30.