



Ihsan Rizal <ihsan.rizal@gmail.com>

Fwd: Please edit your submission

M. Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
To: Ihsan <ihsan.rizal@gmail.com>

Tue, Sep 2, 2025 at 10:19 AM

Begin forwarded message:

From: Journal Of Taibah University Medical Sciences <em@editorialmanager.com>
Date: 2 September 2025 at 07.55.38 GMT+7
To: Moehamad Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
Subject: Please edit your submission
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Re:

Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens

Dear Dr Roeslan,

Your submission entitled "In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens" has been received by Journal of Taibah University Medical Sciences.

However, before we can proceed with the review process we ask you to address the following:

Please provide a complete statement for Ethical Approval. Please edit and resubmit.
If there is an no Ethical approval- the statement should contain there is no ethical issue.

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4. Provide or modify the item/information as requested.
5. Go to "Attach Files" and "Build PDF for my Approval".
6. View and Approve your new PDF file including the changed item(s), or if needed, Edit again.

Thank you for submitting your work to the journal, and if you have any questions, please don't hesitate to contact me.

Yours sincerely,

Journal of Taibah University Medical Sciences

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Ihsan Rizal <ihsan.rizal@gmail.com>

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Tue, Sep 2, 2025 at 12:44 PM

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Subject: Your PDF has been built and requires approval
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Journal of Taibah University Medical Sciences
Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Authors: Muhammad Ihsan Rizal; Syafia Husain; Komariah Komariah; Ciptadhi Trioka Binartha; Arief Cahyanto; Moehamad Orliando Roeslan

Dear Dr Moehamad Orliando Roeslan,

The PDF for your submission, "In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens" has now been built and is ready for your approval. Please view the submission before approving it, to be certain that it is free of any errors. If you have already approved the PDF of your submission, this e-mail can be ignored.

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Kind regards,
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Ihsan Rizal <ihsan.rizal@gmail.com>

Fwd: Editor handles JTUMED-D-25-00786

M. Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
To: Ihsan <ihsan.rizal@gmail.com>

Wed, Sep 3, 2025 at 10:13 PM

Begin forwarded message:

From: Journal Of Taibah University Medical Sciences <em@editorialmanager.com>
Date: 3 September 2025 at 18.34.40 GMT+7
To: Moehamad Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
Subject: Editor handles JTUMED-D-25-00786
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Ms. Ref. No.: JTUMED-D-25-00786
Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal of Taibah University Medical Sciences

Dear Dr Moehamad Orliando Roeslan,

Your submission "In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens" will be handled by Deputy Editor Walaa Abdullah Mumena, PhD.

You may check on the progress of your paper by logging on to the Editorial Manager as an author.

Thank you for submitting your work to this journal.

Kind regards,

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Journal of Taibah University Medical Sciences

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Ihsan Rizal <ihsan.rizal@gmail.com>

Fwd: A manuscript number has been assigned: JTUMED-D-25-00786

M. Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
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Wed, Sep 3, 2025 at 10:14 PM

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Subject: A manuscript number has been assigned: JTUMED-D-25-00786
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Ms. Ref. No.: JTUMED-D-25-00786
Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal of Taibah University Medical Sciences

Dear Dr Moehamad Orliando Roeslan,

Your submission "In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens" has been assigned manuscript number JTUMED-D-25-00786.

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Ihsan Rizal <ihsan.rizal@gmail.com>

Fwd: Editor handles JTUMED-D-25-00786

M. Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
To: Ihsan <ihsan.rizal@gmail.com>

Thu, Sep 4, 2025 at 2:55 PM

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To: Moehamad Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
Subject: Editor handles JTUMED-D-25-00786
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Ms. Ref. No.: JTUMED-D-25-00786
Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal of Taibah University Medical Sciences

Dear Dr Moehamad Orliando Roeslan,

Your submission "In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens" will be handled by Associate Editor Danya Hashem, BDS, MSc, PhD, FHEA.

You may check on the progress of your paper by logging on to the Editorial Manager as an author.

Thank you for submitting your work to this journal.

Kind regards,

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Ihsan Rizal <ihsan.rizal@gmail.com>

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Mon, Sep 8, 2025 at 9:04 AM

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Date: 8 September 2025 at 03:11:27 GMT+7
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Subject: Track the status of your submission to Journal of Taibah University Medical Sciences

Manuscript Number: JTUMED-D-25-00786
Manuscript Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal: Journal of Taibah University Medical Sciences

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Ihsan Rizal <ihsan.rizal@gmail.com>

Fwd: Your Submission - JTUMED-D-25-00786

M. Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
To: Ihsan <ihsan.rizal@gmail.com>

Tue, Oct 21, 2025 at 3:22 PM

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From: Journal Of Taibah University Medical Sciences <em@editorialmanager.com>
Date: 21 October 2025 at 12.55.39 GMT+7
To: Moehamad Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
Subject: Your Submission - JTUMED-D-25-00786
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

CC: "Muhammad Ihsan Rizal" ihsan.rizal@trisakti.ac.id, "Syafia Husain" syafia.husain2@gmail.com, "Komariah Komariah" komariah@trisakti.ac.id, "Ciptadhi Trioka Binartha" cipthadi.trioka@trisakti.ac.id, "Arief Cahyanto" a.cahyanto@ajman.ac.ae

Ms. Ref. No.: JTUMED-D-25-00786

Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal of Taibah University Medical Sciences

Dear Dr Moehamad Orliando Roeslan,

Journal has received the reviewer comments and they recommend reconsideration of your manuscript following revision and modification.

If you feel that you can suitably address the reviewers' comments (included below), I invite you to revise and resubmit your manuscript by Nov 04, 2025.

Kindly revise the manuscript by addressing the reviewers' comments or providing suitable rebuttals for any comments not addressed. You need to highlight the corrections in the text and provide a letter of response by writing point-by-point responses to all comments.

To submit your revision, please do the following:

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4. Click [Submissions Needing Revision]

I look forward to receiving your revised manuscript.

Yours sincerely,

Walaa Abdullah Mumena, PhD
Deputy Editor
Journal of Taibah University Medical Sciences

Reviewers comments:

Deputy Editor Comments:

Thank you for your interest in publishing your work in JTUMED. Please add a dedicated section that clearly presents the strengths and limitations of the study. The Discussion section is currently very brief; all important aspects of the findings should be elaborated on to expand and strengthen this section.

In addition, kindly revise the Conclusion section to include the following:

1. Main findings (1–2 sentences)
2. Recommendations for practice (1–2 sentences)

3. Future research directions

Reviewer #1: This research is direct and straightforward. The study aim and English writing are clear. There is potential for future clinical application. However, the major weakness of this study is its insufficient completeness. It is regarded as a preliminary study and deserves more investigations. Major and minor comments, listed as follow, should be answered or revised.

Major comments:

1. M&M: There is no description nor information about two important positive controls. The authors should carefully revise the M&M section, and make the experiments reproducible for other researchers.
2. M&M: All the important software and materials should have source information in parentheses . For example: company name, city and country names. The authors should follow the Author Guide of this journal. The dosage of the tested chemicals in the experiments should also be clearly displayed.
3. M&M: The authors should clearly describe how many times they repeat the experimental procedures; how they obtained the tested specimens or samples or chemicals. In conclusion, the manuscript should be clear and detail enough to allow other researchers reproduce the experiments.

Minor comments:

1. Abstract: "Factor H-binding protein" should be "factor H-binding protein".
2. Abstract: (alstonine,....., and villalstonine) should move to be after "phytochemicals", instead of after *Alstonia scholaris*.
3. Abstract: The important information of positive controls is absent in the Methods.
4. Line 23 &24, Introduction: "Factor H" should be "factor H".
5. Discussion: The authors should add a paragraph about the weakness of this study. Strictly speaking, the study is not yet complete, because no functional assays were designed and executed for the three phytochemicals.
6. References: The formats of the listed references are inconsistent, regarding upper- and lower-cases of the titles, and abbreviations of the journal names. Please follow the Author Guide and carefully revise each reference.

Reviewer #2: The Manuscript will benefit as per revision with the comments given, Good Luck

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Review Taibah University.docx

17K

TITLE : In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens

The manuscript justifies the research question by the problem and the need for the study of three phytochemicals in *A. scholaris* by in silico molecular docking of periodontal pathogens *P. gingivalis* and *T. denticola*, alstonine, echitamine chloride, and villalstonine against the HmuY receptor in *P. gingivalis* and the Factor H-binding protein (FhbB) in *T. denticola*.

The research adds the importance by connecting the study to periodontitis and to antimicrobial resistance while also addressing an identified knowledge gap related to *A. scholaris*.

Novelty :

The work presents a specific, under-investigated area of research in the field of periodontics.

The work is aimed at two very specific and important virulence factors i.e The HmuY receptor of *P. gingivalis*, which is necessary for survival of the pathogen through heme acquisition and The Factor H-binding protein (FhbB) of *T. denticola*, which protects the microbe from host immune system

Methodology

Various validation steps were conducted in this study

1. Receptor Conformation Check: The Ramachandran plot analysis of the protein receptors confirmed their conformational suitability which were well below the threshold (0.6% for 3H8T and 0% for 3F2V).

2. Redocking and RMSD Calculation: Native ligands were redocked with GOL for 3H8T and FMN for 3F2V while RMSD calculations were performed .

The RMSD measurements of 1.821 Å and 0.851 Å which fall below the accepted threshold of 2.5 Å demonstrate consistent redocking accuracy. The steps maintain that the docking software can accurately predict ligand binding poses. Authors focused on two specific virulence factors that have defined protein databank identifiers: HmuY from *P. gingivalis* (PDB ID: 3H8T) and FhbB from *T. denticola* (PDB ID: 3F2V).

The validation procedure for the 3H8T receptor (*P. gingivalis* HmuY) represents a potential methodological issue. Heme (HEM) served as the functional ligand .. However a much smaller molecule glycerol (GOL) was selected as the ligand for redocking validation. The rationale for this choice given is that GOL "was resolved with clear coordinates in the deposited structure, enabling RMSD calculation" . It is unclear that using a small, simple molecule such as glycerol can provide a strong validation of a docking protocol for such a large and complex binding pocket. The docking may be more or less accurate for small vs. large molecules. the decision to employ glycerol for validation of the docking protocol rather than the physiologically relevant heme ligand is questionable.

In silico methodology cannot directly assess important real-world parameters such as the ability of phytochemicals to reach subgingival sites, their stability in the oral environment, their absorption and/or potential toxicity to human cells. This can be addressed as a limitation.

RESULTS

The first para of the section duplicates the final paragraph in the Method section.. This is a major structural error in the manuscript and shows a lack of careful editing. The "Results" section should contain the results, not a restatement of how they were derived.

Discussion :

The manuscript will benefit from a detailed examination of the kinds of interactions that occurred. The analysis would benefit from an in-depth examination of these compounds' binding mechanisms. The analysis should include details about how hydrogen bonds interact with residues such as TRP70 and TYR116. The analysis would benefit from a biochemical explanation beyond simple numeric comparisons.

A direct comparison with results from other in silico and in vitro studies of alkaloids or other compounds targeting HmuY or FhbB proteins will enhance the discussion if those studies are available.

Villalstonine demonstrates moderate affinity with a measured ΔG value for binding to HmuY. Since it was among the main three compounds studied its findings and potential require more extensive discussion or at least a rationale for its unsatisfactory performance.

Response to Deputy Editor:

Dear Deputy Editor,

Thank you for your comments and suggestions on our manuscript. Below, we provide clarifications and corrections in our response.

Comment 1:

Please add a dedicated section that clearly presents the strengths and limitations of the study.

Response:

We appreciate this suggestion. A concise paragraph on **Strengths and Limitations** has been added at the end of the *Discussion* section. It highlights the validated docking accuracy, the focus on specific virulence factors, and acknowledges that *in silico* results require further biological validation. The toxicity aspect was **not repeated here**, as it has been thoroughly addressed and published in a **separate study** involving *A. scholaris* phytochemicals.

Comment 2:

The Discussion section is currently very brief; all important aspects of the findings should be elaborated on to expand and strengthen this section.

Response:

We have expanded the *Discussion* to include more detailed interpretation of ligand–residue interactions (TRP70, TYR116, LYS101) and a concise comparison with previous *in silico* and antimicrobial studies. However, as this article is submitted under the **Brief Report** category (maximum 1,500 words), the expansion was made concisely to comply with the journal's format requirements while maintaining scientific completeness.

Comment 3:

Revise the Conclusion section to include (1) main findings, (2) recommendations for practice, and (3) future research directions

Response:

The *Conclusion* section has been revised to clearly summarize the main findings, emphasize the potential adjunctive role of *A. scholaris* compounds in periodontal therapy, and suggest future **in vitro** and **in vivo** studies to confirm these computational predictions.

Response to Reviewer #1:

Dear Reviewer,

Thank you for your comments and suggestions on our manuscript. Below, we provide clarifications and corrections in our response.

Comment 1:

M&M: There is no description nor information about two important positive controls. The authors should carefully revise the M&M section and make the experiments reproducible for other researchers.

Response:

We appreciate the reviewer's valuable observation. The revised Methods section now includes complete descriptions of both positive controls.

Comment 2:

M&M: All the important software and materials should have source information in parentheses. For example: company name, city and country names. The authors should follow the Author Guide of this journal. The dosage of the tested chemicals in the experiments should also be clearly displayed.

Response:

We appreciate the reviewer's insightful comment, we have added the company name, city, and country for all software and materials used in the *Methods* section. However, for *in silico* docking, the concentrations were not applicable.

Comment 3:

M&M: The authors should clearly describe how many times they repeat the experimental procedures; how they obtained the tested specimens or samples or chemicals. In conclusion, the manuscript should be clear and detail enough to allow other researchers reproduce the experiments

Response:

We appreciate the reviewer's comment. According to the *AutoDock User Guide* (Garrett M. Morris et al., 2014), reproducibility of *in silico* docking is ensured through the use of documented random seeds, parameter files, and detailed log outputs rather than through manual repetition of the entire procedure. Therefore, we did not repeat the docking experiments separately; instead, each docking job consisted of multiple genetic algorithm (GA) runs ($n = 100$) within AutoDock, as recommended in the official documentation. The input and output files, software versions, and all docking parameters have been reported in the *Materials and Methods* section, enabling full reproducibility by other researchers.

Comment 4:

Abstract: "Factor H-binding protein" should be "factor H-binding protein"

Response:

Corrected as suggested.

Comment 5:

Abstract: (alstonine,....., and villalstonine) should move to be after "phytocompounds", instead of after *Alstonia scholaris*.

Response:

Corrected as suggested.

Comment 6:

Abstract: The important information of positive controls is absent in the Methods.

Response:

The Abstract now indicates that minocycline and chlorhexidine were used as positive controls.

Comment 7:

Line 23 &24, Introduction: "Factor H" should be "factor H".

Response:

Both issues have been corrected

Comment 8:

Discussion: The authors should add a paragraph about the weakness of this study. Strictly speaking, the study is not yet complete, because no functional assays were designed and executed for the three phytochemicals.

Response:

A short paragraph has been added at the end of the Discussion addressing the study's limitations.

Comment 9:

References: The formats of the listed references are inconsistent, regarding upper- and lower-cases of the titles, and abbreviations of the journal names. Please follow the Author Guide and carefully revise each reference.

Response:

All references have been revised according to the JTUMED Vancouver style, with uniform formatting, capitalization, and bold journal names and years

Response to Reviewer #2:

Dear Reviewer,

Thank you for your comments and suggestions on our manuscript. Below, we provide clarifications and corrections in our response.

Comment 1:

The validation procedure for the 3H8T receptor (*P. gingivalis* HmuY) represents a potential methodological issue. Heme (HEM) served as the functional ligand. However a much smaller molecule glycerol (GOL) was selected as the ligand for redocking validation. The rationale for this choice given is that GOL "was resolved with clear coordinates in the deposited structure, enabling RMSD calculation" . It is unclear that using a small, simple molecule such as glycerol can provide a strong validation of a docking protocol for such a large and complex binding pocket. The docking may be more or less accurate for small vs. large molecules. the decision to employ glycerol for validation of the docking protocol rather than the physiologically relevant heme ligand is questionable.

Response:

We thank the reviewer for this important observation. . In the deposited crystal structure 3H8T, the HmuY receptor was determined at high resolution (1.8 Å) and includes heme (HEM) as the physiological ligand. However, the structure also contains glycerol (GOL) molecules that are resolved with well-defined atomic coordinates near the heme-binding pocket, while heme shows partial occupancy and complex metal coordination. Because successful RMSD-based validation requires a ligand with precisely defined experimental coordinates, GOL was selected as a technical reference ligand to evaluate the ability of the docking protocol to reproduce experimentally observed poses under controlled conditions. GOL provides a clear and reproducible benchmark for grid definition, scoring stability, and algorithmic accuracy. Importantly, this validation step was not intended to represent the biological binding event, but to confirm the internal consistency and precision of the docking workflow prior to the actual docking of physiologically relevant ligands. This approach has been used in several computational studies where the native cofactor has ambiguous or incomplete electron density.

Comment 2:

In silico methodology cannot directly assess important real-world parameters such as the ability of phytochemicals to reach subgingival sites, their stability in the oral environment, their absorption and/or potential toxicity to human cells. This can be addressed as a limitation.

Response:

A short paragraph has been added at the end of the Discussion addressing the study's limitations.

Comment 3:

The first para of the section duplicates the final paragraph in the Method section.. This is a major structural error in the manuscript and shows a lack of careful editing. The "Results" section should contain the results, not a restatement of how they were derived

Response:

We appreciate the reviewer's observation. The duplicated paragraph at the start of the Results section has been removed, ensuring that the Results now report only the study findings, while the methodological descriptions remain in the Methods section. This revision enhances the manuscript's organization and readability.

Comment 4:

The manuscript will benefit from a detailed examination of the kinds of interactions that occurred. The analysis would benefit from an in-depth examination of these compounds' binding mechanisms. The analysis should include details about how hydrogen bonds interact with residues such as TRP70 and TYR116. The analysis would benefit from a biochemical explanation beyond simple numeric comparisons.

Response:

We sincerely thank the reviewer for this insightful suggestion. In the revised manuscript, we have expanded the molecular docking analysis to include a detailed discussion of the types of interactions formed between the most active compounds and the key receptor residues.

Comment 5:

A direct comparison with results from other *in silico* and *in vitro* studies of alkaloids or other compounds targeting HmuY or FhbB proteins will enhance the discussion if those studies are available.

Response:

We thank the reviewer for this valuable suggestion. In response, we have expanded the Discussion section, however none appear to directly studies that investigate alkaloids or other compounds specifically targeting the HmuY (of *Porphyromonas gingivalis*) or FhbB (of *Treponema denticola*) with full *in silico* + *in vitro* validation of those exact scaffolds.

Comment 5:

Villalstonine demonstrates moderate affinity with a measured ΔG value for binding to HmuY. Since it was among the main three compounds studied its findings and potential require more extensive discussion or at least a rationale for its unsatisfactory performance.

Response:

We thank the reviewer for this valuable observation. We have expanded the Discussion section to include a rationale for the moderate binding affinity of villalstonine.



Ihsan Rizal <ihsan.rizal@gmail.com>

Fwd: Revision reminder for Journal of Taibah University Medical Sciences

M. Orliando Roeslan <orliando.roeslan@trisakti.ac.id>
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Tue, Oct 28, 2025 at 1:58 PM

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Manuscript Number: JTUMED-D-25-00786
In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens

Dear Dr Roeslan,

We would like to remind you that on Oct 21, 2025 we asked you to revise your above referenced manuscript and your revision is due by Nov 04, 2025.

Journal of Taibah University Medical Sciences values your contribution and we look forward to receiving your revised manuscript.

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Ihsan Rizal <ihsan.rizal@gmail.com>

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Subject: Editor handles your revised submission JTUMED-D-25-00786R1
Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Ref.: Revision of JTUMED-D-25-00786R1
Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens

Dear Dr Roeslan,

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Ihsan Rizal <ihsan.rizal@gmail.com>

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Manuscript Number: JTUMED-D-25-00786
Manuscript Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal: Journal of Taibah University Medical Sciences

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Ihsan Rizal <ihsan.rizal@gmail.com>

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Reply-To: Journal Of Taibah University Medical Sciences <support@elsevier.com>

Ms. Ref. No.: JTUMED-D-25-00786R1
Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal of Taibah University Medical Sciences

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Ihsan Rizal <ihsan.rizal@gmail.com>

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Title: In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens
Journal of Taibah University Medical Sciences

Dear Dr Moehamad Orliando Roeslan,

I am pleased to inform you that your paper "In silico Evaluation of Alstonia scholaris Phytochemicals Against Periodontal Pathogens" has been accepted for publication in Journal of Taibah University Medical Sciences.

Thank you for submitting your work to Journal of Taibah University Medical Sciences.

Yours sincerely,

Walaa Abdullah Mumena, PhD
Deputy Editor
Journal of Taibah University Medical Sciences

Comments to Authors:

Reviewer #1: The authors have revised the manuscript accordingly and sufficiently.

Reviewer #2: All comments have been addressed . There appears to be one typo mistake in Table 2 .
eg TRP70 dan TYR116 — dan appears many times in the table / replace "dan" with "and"

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