

### Review Form 3

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| Journal Name:            | <a href="#">South Asian Research Journal of Natural Products</a>   |
| Manuscript Number:       | Ms_SARJNP_128674   |
| Title of the Manuscript: | In Silico Molecular Docking Studies of the Phytochemicals from Azadirachta indica Stem Bark Against Alpha-Amylase for Management of Type 2 Diabetes. |
| Type of the Article      | Research Article   |

#### **General guidelines for the Peer Review process:**

This journal's peer review policy states that **NO** manuscript should be rejected only on the basis of '**lack of Novelty**', provided the manuscript is scientifically robust and technically sound. To know the complete guidelines for the Peer Review process, reviewers are requested to visit this link:

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#### **PART 1: Comments**

|   | Reviewer's comment  | Author's Feedback (Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here) |
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| <b>Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.</b> | <ul style="list-style-type: none"><li>- This study investigates the antidiabetic potential of phytochemicals extracted from the stem bark of <i>Azadirachta indica</i> using molecular docking against the <math>\alpha</math>-amylase enzyme.</li><li>- GC-MS analysis identified 20 compounds, including Resveratrol and Indazol-4-one, 3,6,6-trimethyl-1-phthalazin-1-yl-1,5,6,7-tetrahydro-, which exhibited binding energies of -8.0 and -9.4 kcal/mol, respectively, surpassing the control drug Acarbose (-8.5 kcal/mol).</li><li>- The compounds with high binding affinities adhered to Lipinski's rule of five, demonstrating drug-likeness.</li><li>- These findings highlight the potential of <i>A. indica</i> stem bark as a source of bioactive compounds for managing type 2 diabetes, offering promising candidates for future drug development.</li></ul> |  |
| <b>Is the title of the article suitable? (If not please suggest an alternative title)</b>   | <p>The current title, "In Silico Molecular Docking Studies of the Phytochemicals from <i>Azadirachta indica</i> Stem Bark Against Alpha-Amylase for Management of Type 2 Diabetes," is informative but slightly lengthy. It effectively communicates the focus of the study, but a more concise alternative could improve readability and impact.</p> <p>- <b>Suggested Alternative Title:</b><br/>"Molecular Docking of <i>Azadirachta indica</i> Stem Bark Phytochemicals Against <math>\alpha</math>-Amylase for Type 2 Diabetes Management"</p>   |  |

**Review Form 3**

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|---|---|--|
| <p><b>Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here.</b></p> | <p>The abstract is comprehensive and clearly outlines the objective, methods, key findings, and potential significance of the study. However, a few minor adjustments could improve its clarity and conciseness:<br/> <b>Introduction/Context:</b> The opening sentence could be shortened to better focus on the main issue. For example, rather than stating "Diabetes mellitus–associated health complications and the issue of drug resistance have significant challenges for pharmacists and research scientists," you could reframe it as, "Diabetes mellitus and drug resistance pose significant challenges in treatment."<br/> <b>Methods:</b> The sentence "In this study, the phytochemicals in the stem bark of the plant sample was extracted with chloroform and the compounds present were identified using gas chromatography-mass spectrometry" could be revised to improve <b>clarity</b>. Consider: "In this study, phytochemicals from the stem bark of <i>Azadirachta indica</i> were extracted using chloroform and identified via gas chromatography-mass spectrometry."<br/> <b>Results:</b> The results section could briefly mention the number of compounds identified and their relevance to the antidiabetic activity, providing a more holistic view of the findings.<br/> <b>Conclusions:</b> The abstract currently ends by focusing on the two compounds with good binding affinity. It might be useful to briefly suggest their potential for further investigation or application, e.g., "These findings suggest that these compounds could serve as promising candidates for further drug development against type 2 diabetes mellitus."<br/> <b>- Revised Abstract:</b><br/> Diabetes mellitus and drug resistance pose significant challenges in treatment. Crude extracts from plants, such as <i>Azadirachta indica</i>, which is known for its medicinal properties, could offer alternative agents for diabetes management. However, the specific bioactive compounds responsible for its antidiabetic activity remain poorly understood. In this study, phytochemicals from the stem bark of <i>Azadirachta indica</i> were extracted using chloroform and identified by gas chromatography-mass spectrometry (GC-MS). The antidiabetic potential of these compounds was assessed through <i>in silico</i> molecular docking against the enzyme <math>\alpha</math>-amylase. The results showed that the binding free energy of Indazol-4-one, 3,6,6-trimethyl-1-phthalazin-1-yl-1,5,6,7-tetrahydro- (-9.4 kcal/mol) had a better binding affinity than the control drug Acarbose (-8.5 kcal/mol), while Resveratrol (-8.0 kcal/mol) showed a similar affinity to Acarbose. Both compounds adhered to Lipinski's rule, demonstrating drug-likeness and highlighting their potential as drug candidates for type 2 diabetes mellitus treatment.<br/> <b>- Suggestions for Keywords:</b><br/> Consider revising "Alpha – amylase" to "<math>\alpha</math>-amylase" for consistency in formatting.</p> |  |
| <p><b>Is the manuscript scientifically, correct? Please write here.</b></p>   | <p>The manuscript appears to be scientifically correct.</p>   |  |
| <p><b>Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.</b></p>                         | <p>The references in the manuscript are generally comprehensive and cover a range of topics related to diabetes, its treatment, and molecular docking studies.</p>  |  |
| <p><b>Is the language/English quality of the article suitable for scholarly communications?</b></p>   | <p>The overall language quality of the manuscript is generally understandable, but there are a few areas where improvements can be made to enhance clarity, coherence, and professionalism, particularly for scholarly communication.</p>   |  |
| <p><b>Optional/General</b> comments</p>   | <p>Overall, this is a well-conducted study with valuable findings that contribute to the field. With some minor revisions in clarity, structure, and precision, the manuscript could be strengthened for publication. The authors have done a good job in presenting their research, and with a few improvements, this study has great potential for scientific dissemination.</p>  |  |

**PART 2:**

|  | Reviewer's comment  | Author's comment (if agreed with reviewer, correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here) |
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| <p><b>Are there ethical issues in this manuscript?</b></p> | <p><i>(If yes, Kindly please write down the ethical issues here in details)</i></p> |   |

**Reviewer Details:**

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|---|---|
| <p>Name:</p>                                | <p><b>Gheraissa Noura</b></p>                           |
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