

Review Form 3

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| Journal Name: | Journal of Pharmaceutical Research International |
| Manuscript Number: | Ms_JPRI_126154 |
| Title of the Manuscript: | Prediction of Lead Molecule esculetin of Tridax procumbens against zika virus envelope protein |
| Type of the Article | Original Research Article |

Review Form 3

PART 1: Review Comments

| Compulsory REVISION 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) |
|---|---|---|
| <p>Please write a few sentences regarding the importance of this manuscript for the scientific community. Why do you like (or dislike) this manuscript? A minimum of 3-4 sentences may be required for this part.</p> | <p>This manuscript explores the interaction of flavonoids from <i>Tridax procumbens</i>, specifically esculetin, with the Zika virus, an area of great importance given the absence of an effective vaccine for the virus. The use of in silico methods provides valuable insights into the binding mechanisms between the compounds and the viral envelope protein. The integration of Ayurinformatics is a novel approach that bridges ancient therapeutic knowledge with modern drug discovery. While the manuscript offers significant insights, incorporating binding free energy calculations could further strengthen the study's findings.</p> | |
| <p>Is the title of the article suitable? (If not please suggest an alternative title)</p> | <p>Yes it is.</p> | |
| <p>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.</p> | <p>The abstract provides a broad overview, but it lacks focus and clarity. It mentioned Siddha, Ayurveda, and Ayurinformatics without directly connecting them to the core of the study, which is the in silico exploration of compounds from <i>Tridax procumbens</i> for Zika virus treatment. The abstract could benefit from mentioning the methods and key results in a precise way.</p> | |
| <p>Are subsections and structure of the manuscript appropriate?</p> | <p>Yes, It is.</p> | |
| <p>Please write a few sentences regarding the scientific correctness of this manuscript. Why do you think that this manuscript is scientifically robust and technically sound? A minimum of 3-4 sentences may be required for this part.</p> | <p>The study perform shows a novelty in term exploring computational techniques such as molecular docking and molecular dynamic simulation that was used to investigate the interactions between <i>Tridax procumbens</i> flavonoids and the Zika virus envelope protein. The use of in silico approaches like SYBYL-X software, along with ADME and toxicity profiling, aligns with standard practices in early-stage drug discovery. The selection of esculetin and procumbenetin as lead molecules is based on their known pharmacological properties, making the study's approach well-founded. However, incorporating further analyses, such as binding free energy calculations (e.g., MMGBSA or MMPBSA), would enhance the understanding of the interaction dynamics and provide a more comprehensive evaluation of the compounds' potential as drug candidates.</p> | |
| <p>Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form. =</p> | <p>The references stated in the manuscript are relatively recent and relevant. However, adding more references, particularly from the last few years, would provide a broader context and further strengthen the scientific foundation of the study. For example, Since Ayurinformatics is a novel field, it would be helpful to reference recent works that discuss the integration of traditional medicine with bioinformatics approaches.</p> | |
| <p>Minor REVISION comments</p> <p>Is the language/English quality of the article suitable for scholarly communications?</p> | <p>The language use are suitable but there some grammar errors in the manuscripts such as "Several biological active compounds of herbs were isolated and involved in various pharmacological activities".</p> | |
| <p>Optional/General comments</p> | <p>Overall, the study is novel. However, incorporating the suggested analyses, such as binding free energy calculations (e.g., MMGBSA or MMPBSA), and including more recent references, would strengthen the findings and provide a more comprehensive evaluation of the interactions between the flavonoids and the Zika virus envelope protein.</p> | |

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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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| Are there ethical issues in this manuscript? | <i>(If yes, Kindly please write down the ethical issues here in details)</i> | |

Reviewer Details:

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