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Peer Review Reports

Immunoinformatics designing of peptide-based vaccine for malaria infection

The article went through 4 rounds of review and 1 of the 3 reviewers agreed in advance to publish their review reports without disclosing their identity.

The authors agreed to disclose the reviewers' reports and their responses to the reviewers' comments.

Disclaimer: The peer review report content is the entire copy of the reviewers' and authors' comments. Typing and punctuation errors are not edited.

ROUND 1

Reviewer A: The reviewer did not allow the publication of the reports
Recommendation: Revisions Required

No Reviewer Files

Reviewer B: The reviewer did not allow the publication of the reports
Recommendation: Resubmit for Reviewer

No Reviewer Files

Reviewer C: Anonymous
Recommendation: Revisions Required

#1. The results of the validation of the protein structure present a good part of the amino acid residues outside the permitted region, based on the Ramachandran graph. How do the authors justify the validation of the model?

#two. The interpretation of the results on the characterization of the protein structure carried out in PROCHECK and the molecular dynamics carried out in iMODS lacks references from previous studies that use this prediction model. Authors must compare (positively or negatively) other references from previous studies to validate the findings.

#3. Some texts between figures are very short, authors should relocate the figures to an ideal location that follows the flow of the text.

#4. Do the authors have a record of the quaternary structure? It would be ideal to show a three-dimensional structure of the quaternary structure or to show results of a possible homology modeling.

#5. Figure 6d can easily be converted into a table.

#6. Authors must demonstrate whether the molecular docking simulation model is of the protein-protein or ligand-protein type.

#7. How do the authors justify affinity energies around -300 (kcal/mol?)? What is the unit of affinity energy? Is this a relative or absolute value? The discussion of molecular docking was not clear.
Reviewer Files

ROUND 2

Reviewer A: The reviewer did not allow the publication of the reports
Recommendation: Accept Submission

No Reviewer Files

Reviewer B: The reviewer did not allow the publication of the reports
Recommendation: Accept Submission

No Reviewer Files

Reviewer C: Anonymous
Recommendation: Revisions Required

#1. The authors' aim is to develop a new peptide-based therapy but they do not elucidate the 2D structure of the compounds. I recommend that the authors show these structures.

#2. To validate the peptide model, it is recommended that the authors carry out molecular docking simulations, as well as validating the structure of the antigen protein.

#3. Figure 1 is still of dubious quality. I suggest that the authors reformulate it to a quality that is ideal for reading, including the steps suggested in this review. Check the resolution of the other figures.

#4. I suggest that the authors describe the methodological diagram briefly, including a reference that suggests the reproducibility of the methodological model to which this study was adapted.

#5. Figure 2 is not self-explanatory. In it, abbreviations should be avoided and better explained, so that the reader doesn't need to look up what they mean in the text, but should refer to the text only to delve deeper into the model.

#6. In the topic “3.4 Physicochemical properties of the vaccine construct”, what pharmaceutical and medicinal criteria do these vaccine structures meet? Use this information to support your findings on the physicochemical properties.

#7. The authors should carry out homology modeling (e.g. SwissMODEL) to estimate the quaternary structure of the protein. This should be the starting point for molecular docking simulations with peptide structures. I recommend carrying out this protocol for better structural elucidation of the peptides an.
Reviewer Files

ROUND 3

Reviewer C: Anonymous
Recommendation: Decline Submission

The comments have not been properly resolved. In this case, I must recommend rejection of this work.
No Reviewer Files

ROUND 4

Reviewer C: Anonymous
Recommendation: Accept Submission

Here is my current opinion on the review of the article entitled IMMUNOINFORMATICS DESIGNING OF PEPTIDE- BASED VACCINE FOR MALARIA INFECTION

Regarding the molecular dynamics simulations, the figures representing the results remain of low quality, even after several rounds of review, but the methodological flowcharts have improved considerably. The reviews were carried out almost completely, so I must recommend the acceptance of this work.
NOTE: Disregard the previous review!
Best regards
No Reviewer Files

ARTICLE ACCEPTED