

### Review Form 3

Journal Name:	<a href="#">Current Journal of Applied Science and Technology</a>
Manuscript Number:	Ms_CJAST_130593
Title of the Manuscript:	Performing effective calculations of protein - ligand binding free energy with the help of molecular dynamics methods
Type of the Article	Research

#### PART 1: Comments

	Reviewer's comment	Author's Feedback <i>(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)</i>
<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>	1. It may be helpful for drug discovery and development, mainly for Factor Xa inhibitors. 2. The manuscript may contribute valuable applications and findings in molecular dynamics. 3. The experimental data, observations are quite relevant to the current study. 4. Provides a comprehensive study.	Thanks for your comments.
<b>Is the title of the article suitable? (If not please suggest an alternative title)</b>	Yes	Thanks for your comments.
<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>	YES, It may include most relevant results as well.	Thanks for your comments.
<b>Is the manuscript scientifically, correct? Please write here.</b>	YES, The manuscript effectively summarizes the findings.	Thanks for your comments..
<b>Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.</b>	YES, But some recent references may be added.	Thanks for your comments.  One paper using machine learning models and molecular dynamics studies dated in 2022 have been added to references. (Akkus, E., Tayfuroglu, O., Yildiz, M., & Kocak, A. (2022). Accurate binding free energy method from end-state MD simulations. Journal of Chemical Information and Modeling, 62(17), 4095-4106.)
<b>Is the language/English quality of the article suitable for scholarly communications?</b>	Yes	Thanks for your comments.
<b><u>Optional/General</u> comments</b>	1. Minor grammatical corrections.	Thanks for your comments.  Minor typo mistakes and grammatical corrections have been made. All the corrections were marked with a yellow highlighter. Strikethrough words will be deleted in the final version of the manuscript after your review.  "Binding enery" term updated as "Binding free energy" through the manuscript  "binding pocket" term updated as "binding site resdiues" through the manuscript

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