Review Form 1.6

Journal Name:	**Asian Journal of Chemical Sciences**
Manuscript Number:	**Ms_AJOCS_89860**
Title of the Manuscript:	**Molecular docking, pharmacokinetics and molecular dynamic simulation studies of some bioactive compounds isolated from Entandrophragma congoënse for antiplasmodial activity.**
Type of the Article	**Original Research Article**

General guideline for 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 guideline for Peer Review process, reviewers are requested to visit this link:

(https://www.journalajocs.com/index.php/AJOCS/editorial-policy)

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PART 1: Review Comments

	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)*
Compulsory REVISION comments	Manuscript Number: **Ms_AJOCS_89860** **Molecular docking, pharmacokinetics and molecular dynamic simulation studies of some bioactive compounds isolated from *Entandrophragma congoënse* for antiplasmodial activity.** The authors used the experimental data available in the literature for their molecular modeling, but needs some significant improvements to be recommended for publication. The following recommendation need to be made: 1. the reference must be written in the middle or at the end of the paragraph not at the beginning of the paragraph. 2. authors should add the active site (VAL532, ILE237, LEU531, HIE185, TYR528, ASN274, ARG265) of the protein in the manuscript. In order to evaluate the results of the molecular docking 3. The author did not correctly determine the grid box . By my estimation, the grid should be (X = 19.38, Y = -16.911 and Z = -18.21). In order for the authors to confirm the molecular docking results, they need to validate the molecular docking by the re-docking method. 4. In the molecular dynamics part, the counter ions are in the form of Na^+ alone or Na^+ and cl^- at a concentration of 0.15 M? 5. check that it is Gastro Intestinal Absorption (GIA) or Human Intestinal Absorption, as GIA is not listed on the website http://lmmd.ecust.edu.cn/admetsar2. 6. Binding affinity is not the only indicator of activity. Indeed, high docking scores do not reflect the position and formation of strong interactions with the active site of the protein. Have you checked the interactions with the amino acids of all complexes. 7. check the IC50 of all compounds. I think IC50=0.44 instead of 0.47 for compound L4.. 8. Table 3 should be deleted, as Table 2 clearly shows the type of interaction with the corresponding distances. 9. According to Figure 1, compound L15 should have the lowest value of RMSD. 10. Based on Figure 2, the authors need to identify the amino acid exceeding 1.5 (red), to see if it belongs to the active site or not. 11. The authors must come to a conclusion, because this work deserves a detailed conclusion.	
Minor REVISION comments		
Optional/General comments		

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?	*(If yes, Kindly please write down the ethical issues here in details)*	

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Reviewer Details:

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