

## Review Form 1.6

Journal Name:	<a href="#">Journal of Pharmaceutical Research International</a>
Manuscript Number:	Ms_JPRI_83791
Title of the Manuscript:	Virtual screening to identify protein targets of <i>Aggregatibacter actinomycetemcomitans</i> interacting with emodin
Type of the 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:

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**PART 1: Review Comments**

	<b>Reviewer's comment</b>	<b>Author's comment</b> (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)
<b>Compulsory</b> REVISION comments	<p>The research concerns the <i>in silico</i> search of protein targets of <i>Aggregatibacter actinomycetemcomitans</i> for emodin compound. In general, the idea and the methods used are correct. However, there is work to be done on the Manuscript. Please methodically, organize and describe the methods used in the research (what was the starting point and the next steps). This applies to the description in the Abstract and in the Materials and Methods section.</p>	
<b>Minor</b> REVISION comments	<p>Abstract:</p> <ol style="list-style-type: none"> <li>1. "provides some benefits to the bacterium"- please clarify this statement</li> <li>2. "<b>Results:</b> Peptide epitopes present in the virulence factors were identified using the BepiPred tool"- the phrase so formulated is about Methods, not Results. Please describe only your results here.</li> </ol> <p>Introducion:</p> <ol style="list-style-type: none"> <li>1. The mechanisms by which <i>A. actinomycetemcomitans</i> cause <b>loss of attachment-</b> mental shortcut, please expand.</li> <li>2. Regarding the description of <i>A. actinomycetemcomitans</i> - this species is still under investigation and there are many more recent publications than those cited by the authors (e.g. <a href="https://www.frontiersin.org/articles/10.3389/fimmu.2019.00728/full#B13">https://www.frontiersin.org/articles/10.3389/fimmu.2019.00728/full#B13</a> , <a href="https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6963667/">https://www.ncbi.nlm.nih.gov/pmc/articles/PMC6963667/</a>). Please update the References.</li> <li>3. There is no description of the emodin here. Please introduce the reader to the topic.</li> <li>4. "Our team has extensive knowledge and research experience that has translate into high quality publications (11–23),(24–28) (29) (30)"- It is absolutely necessary to remove this sentence, which does not add anything to the topic of the article, and any citations from References that do not relate to the subject of the study.</li> </ol> <p>Materials and methods:</p> <ol style="list-style-type: none"> <li>1. Sentence" The study aims to screen protein targets in <i>A. actinomycetemcomitans</i> that could possibly interact with emodin" it is an unnecessary repetition here.</li> <li>2. "by VICMPred and VirulentPred" - Provide citations, links to each database used in the study or, for example, VICMPred asks you to cite the following paper if you are using VICMpred: Saha, S. and Raghava, G.P.S. (2006) VICMpred: SVM-based method for the prediction of functional proteins of gram-negative bacteria using amino acid patterns and composition. Genomics Proteomics &amp; Bioinformatics. 4(1):42-7</li> </ol> <p>Results:</p> <ol style="list-style-type: none"> <li>1. You should always describe the results and then refer the reader to Figures or Tables</li> <li>2. Are the demonstrated virulence factors described in the literature?</li> <li>3. "The graph depicts the green colour as avirulent and yellow as virulent"</li> <li>4. "The growth and acid production of <i>S. mutans</i> were significantly inhibited by emodin (0.5–2 mg/ml). Emodin also significantly suppressed the synthesis of insoluble glucans by <i>S. ...</i>" What is this sentence related to? Careless editing.</li> <li>5. "A study (32) reported the process of inhibition by reserpine... and ATP - binding cassette (35,36)" This fragment of the text describes completely different studies, it should be deleted. Citations32-36 can only be added as a supporting to sentences "In silico validation is inevitable while choosing a compound to be tested under in vitro and in vivo conditions. It provides clues about the pathway which can be targeted during preliminary screening (31)".</li> <li>6. Please present Fig. 2 in a better, more distinct way.</li> </ol>	

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Optional/General comments	-	
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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>	

**Reviewer Details:**

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