

Review Form 1.7

Journal Name:	Asian Journal of Biotechnology and Genetic Engineering
Manuscript Number:	Ms_AJBGE_110809
Title of the Manuscript:	In Silico Analysis and Molecular Docking Studies of Potential Adenylyl Cyclase Type 2 Inhibitors Using Oleandrin Glycosides
Type of the Article	

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)
<p>Compulsory REVISION comments</p> <p>1. Is the manuscript important for scientific community? (Please write few sentences on this manuscript)</p> <p>2. Is the title of the article suitable? (If not please suggest an alternative title)</p> <p>3. Is the abstract of the article comprehensive?</p> <p>4. Are subsections and structure of the manuscript appropriate?</p> <p>5. Do you think the manuscript is scientifically correct?</p> <p>6. Are the references sufficient and recent? If you have suggestion of additional references, please mention in the review form.</p> <p>(Apart from above mentioned 6 points, reviewers are free to provide additional suggestions/comments)</p>	<p>Title: In silico analysis and molecular docking studies of potential adenylyl cyclase type 2 inhibitors using Oleandrin glycosides</p> <p>Summary: The study in silico experimental study that models Adenyl Cyclase Type 2 with computational software; it is the Phyre tool, and ligand selection by ChemBioDraw using SMILES drawing and/or common molecule retrieval, and analysis of target active sites using MOEs molecular docking simulation tools and analysis. The Ramach. psi phi angulation plot was also utilized to determine the configuration helical structures; the R. plot of the AC 2ary struct. shows mostly an R-handed alpha-helix with some Beta-pleated sheet. As per the molecule-to-AC enzyme model fit, there are hydrophilic (polar) and non-polar interactions with certain R-groups The Oleandrin glycoside molecule is shown to be a good fit with low RMSE (1.41 - 6.78 _).</p> <p>Assess./Recomm.: There is initial study data analysis and presentation as shown. The Methods and Results sections would need to be more complete, and descriptive statistics ranges (rmsd plus, minus) with also the sampling distribution CI values with Pr for sign., and the correlation values for determining of distribution scores (+/- Z) will result in a complete table. The earlier literat. on the diffraction R (free) reliabiliy-factors (low or high) maybe applicable here. Additional comments: i) Is AC located in juxtaposition to the Na/K ATPase as the selected molecule also fits the Na/K ATPase channel site; and ii) is the cell membrane-assoc. Oleandrin hydrolysis product also fit the model; and iii) is it possible to rank order the affinity constants in percent for the selected molecules. Once there is additional presentation of the study findings, it can be further evaluated.</p>	
<p>Minor REVISION comments</p> <p>1. Is language/English quality of the article suitable for scholarly communications?</p>	The grammar and sentence structure are fine.	
<p>Optional/General comments</p>	As above	

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

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