

Review Form 1.6

Journal Name:	Journal of Pharmaceutical Research International
Manuscript Number:	Ms_JPRI_77193
Title of the Manuscript:	In Silico Molecular Docking Analysis of the Potential role of Reticuline and Coclaurine as Anti-colorectal Cancer Alkaloids
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:

<http://peerreviewcentral.com/page/manuscript-withdrawal-policy>

Review Form 1.6

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>	<ol style="list-style-type: none"> Why the author selects only 2 ligands from the family of the alkaloids and what is the clinical significance of these ligands in cancer? In the abstract section author mention that "the investigated receptors were successfully docked onto reticuline and coclaurine ligands for drug interaction studies" I think ligands docked to receptors, not the receptors docked the ligand. Please correct the sentence. In the manuscript the author didn't define or mention the active sites and residues of the proteins in the manuscript which were taken under consideration for the docking and also make proper reference for the selection of the active sites of the proteins. Accept the binding energies author unable to show any other information of the docking complex like bond information and interacting residues. In the manuscript author mention that "For this study, ligands belong to alkaloid phytochemicals were screened with the specific anti-cancer receptor" were are the results for the virtual screening of the ligands? Please provide the detailed results of the screening of the ligands. (how many ligands you had taken for the study at the start) In section 2.5 Multi-Receptor Docking: In the manuscript mentioned 2 softwares iGEMDOCK and AutoDock vina software were used for the docking but in the result section only one software binding energy was shown; this energy belongs to which software?? In the manuscript author mention two words: Binding energy and docking energy. "On the other hand with respect to Coclaurine ligand the receptors showed less binding energy which were -87.8, -102.3, -76.7, and -96.6 kcal/mol were discovered to represent the docked energies of receptor-ligand complex-1". Both words have different means, please explain them. These PDB IDs do not belong to humans except the last one. So how do you compare the results in a heterogeneous system? <table border="1" data-bbox="1026 1234 1760 1648"> <thead> <tr> <th>Gene name</th> <th>Receptor name</th> <th>PDB id</th> <th>Comments</th> </tr> </thead> <tbody> <tr> <td>TNIK</td> <td>Nck Interacting kinase</td> <td>5CWX</td> <td>This ID does not belong to humans: Xanthomonas oryzae pv. oryzae KACC 10331</td> </tr> <tr> <td>VEGFR</td> <td>Vascular endothelial growth factor</td> <td>1WQ9</td> <td>Daboia russelii russelii</td> </tr> <tr> <td>EGFR</td> <td>Epidermal growth factor receptor</td> <td>3G5X</td> <td>Mus musculus</td> </tr> <tr> <td>AKT2</td> <td>Protein kinase B</td> <td>1MRV</td> <td>Homo sapiens</td> </tr> </tbody> </table>	Gene name	Receptor name	PDB id	Comments	TNIK	Nck Interacting kinase	5CWX	This ID does not belong to humans: Xanthomonas oryzae pv. oryzae KACC 10331	VEGFR	Vascular endothelial growth factor	1WQ9	Daboia russelii russelii	EGFR	Epidermal growth factor receptor	3G5X	Mus musculus	AKT2	Protein kinase B	1MRV	Homo sapiens	
Gene name	Receptor name	PDB id	Comments																			
TNIK	Nck Interacting kinase	5CWX	This ID does not belong to humans: Xanthomonas oryzae pv. oryzae KACC 10331																			
VEGFR	Vascular endothelial growth factor	1WQ9	Daboia russelii russelii																			
EGFR	Epidermal growth factor receptor	3G5X	Mus musculus																			
AKT2	Protein kinase B	1MRV	Homo sapiens																			
<p>Minor REVISION comments</p>	<ol style="list-style-type: none"> The reference was not in a proper format as per the journal guidelines and also check the reference number properly. In the manuscript, Fischer reference is [28] but in the reference section, it is 27. Read all the paragraphs properly to improve the grammar and typo mistakes. Correct reference no.19 all words are in capital letters. 																					

Review Form 1.6

Optional/General comments		

PART 2:

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

Reviewer Details:

Name:	Krishna Pal Singh
Department, University & Country	University of Rostock, Germany