

Book Name:	Advanced Concepts in Pharmaceutical Research
Manuscript Number:	Ms_BP_12271F
Title of the Manuscript:	SYNTHESIS AND MOLECULAR DOCKING STUDIES OF ETHYL 1-BENZENESULFONYL -2-[(E)-2-(2 METHYLPHENYL) ETH HUMAN RENIN COMPLEXED WITH INHIBITOR
Type of the Article	Book Chapter

PART 1: Review Comments

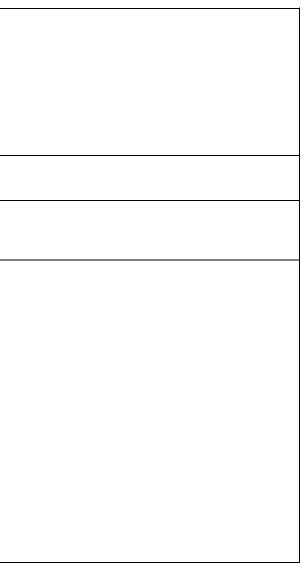
Reviewer's comment	Author's comment(If agreed
	highlight that part in the manu
	here)

THENYL] INDOLE -3-CARBOXYLATE WITH

ed with the reviewer, correct the manuscript and nuscript. Authors must write his/her feedback



Is the manuscript important for the scientific community? Please write a few sentences explaining your answer	This manuscript presents novel indole compounds evaluated for their potential antihypertensive activity through inhibition of renin, a key enzyme in the production of angiotensin II.	
	• The molecular docking studies provide valuable insights into the mechanisms underlying their activity, further enhancing our understanding of their potential efficacy.	
	 This work contributes to the scientific community by expanding the potential of compounds that could be explored for the treatment of hypertension, addressing a critical need for more effective therapeutic options in cardiovascular medicine. 	
Is the title of the article suitable? Do you have any alternative Title in your mind?	I would suggest strongly to authors to change the title to "Synthesis guided by in-silico approaches of "	
Is the abstract of the article comprehensive? If your answer is No, please provide suggestions	Yes, the title looks comprehensive but can be extended more to include other analysis in complement to the molecular docking.	
Do you think the English quality of the article is suitable for scholarly communications? If your answer is No, please provide suggestions	 Some sentence need to be active and concise for eg. ""Docking studies using Molegro Virtual Docker (MVD) on the human Renin complexed with inhibitor (PDB ID: 2IKO) demonstrate its role in the molecule's antihypertensive activity." Ensure parallel structure in phrases or lists. For example, "ReRanking score and binding poses of the molecule" need be revised to "ReRanking scores and binding poses of the molecule" for consistency. Ensure consistent use of tense and formatting throughout the introduction paragraph. For eg, "Currently the hypertension attracts the kidney diseases" need to be revised to "Currently, hypertension is associated with kidney diseases." (ESRD) End stage renal disease: Acronym should be after. Avoidance of repetition: Avoid repeating similar information or ideas, such as the mention of hypertension attracting kidney diseases, unless necessary for emphasis or clarity. same for the sentences here "Compounds having indole groups are biologically important compounds. Indole along with their several derivatives finds a prominent place in synthetic organic chemistry" Missing verbs at lots of places "using Molegro Virtual Docker software was done to understand the basic mechanism of inhibition." 	
	Authors need to review their manuscript carefully to correct these mistakes	





Please provide your comments regarding the appropriateness of different sections of the manuscript.	 Abstract needs to be comprehensive; for eg. after first sentence need to provide details if there has been any success with drug discovery and why its challenging against modulating hypertension Also, improve the transition of sentences from renin inhibitors to "indole" In Introduction: Authors also need to provide more statistical data of hypertension around the world to make the study more visible. They should extend the numbers beyond India to worldwide. Authors need to combine "Importance of indole" section with introduction. Remove multiple and excessive use of "Molegro Virtual Docker" in abstract and introduction. Explain it only in methods section or use MVD where its absolutely necessary. "Docking is frequently used to predict the binding orientation of small drug candidate to their protein targets" there are lots of papers which criticize docking. So correct this sentence to say that "Docking combined with other computational methods is used to predict the binding orientation and affinity" Explain more "Preparation of Ligand Structure": whether hydrogen added and which charges were added. Define the process what changes where made to protein in "Preparation of Protein structure" In the section Active site identification: Instead carry out the same analysis on more than one poses which are in RMSD range of 1-2 Angstrom and then take the average. As ligand is dynamic and MD simulations were not performed; this analysis will provide better scores. Use multiple conformations of binding site or protein or perform loop modeling of protein if there is a loop in the binding pocket and then provide lescores on different loops. Use these two references to implement loop modeling. For method: López-Blanco, José Ramón, et al. "RCD+: Fast loop modeling server." Nucleic acids research 44.W1 (2016): W395-W400. APA For using it: Gupta, Aayush, and H	
Do you think that the references in the manuscript are proper, recent and sufficient? If you have any suggestions, please write here.	Yes need to provide more references based on above comments in introduction and methods. The manuscript needs a major revision.	

PART 2:

		Author's comment(if agreed w highlight that part in the manuse his/her feedback here)
Are there ethical issues in this manuscript?	(If yes, Kindly please write down the ethical issues here in details)	

Reviewer Details:

Name:	Aayush Gupta
Department, University & Country	USA

l with reviewer, correct the manuscript and uscript. It is mandatory that authors should write