<u>**Review Form2**</u>

Book Name:	[Pharmaceutical Research- Recent Advances and Trends](#)
Manuscript Number:	**Ms_BPR_1928**
Title of the Manuscript:	**Development of Scoring-Assisted Generative Exploration and Its Application to Inhibitor Design**
Type of the Article	**Book chapter**

<mark>**PART 1:**</mark> **Review Comments**

<u>Compulsory</u> REVISION comments	Reviewer's comment	Author's Feedback *(Please correct the manuscript and highlight that part in the manuscript. It is mandatory that authors should write his/her feedback here)*
Please write few sentences regarding the importance this manuscript for scientific community. Why do you like (or dislike) this manuscript? Minimum 3-4 sentences may be required for this part.	**This manuscript is discussing methods ofgenerartive exploration emphasizing Score Assisted Generative Exploration,which helps the scientific community field of drug invention by automating the molecular design process,which facilitates the quick proposal of viable drug candidates with affinity,efficacy and safety profiles.These advanced tools and software are contributing to the science especially medical field with many of the positive outcomes.**	
Is the title of the article suitable? **(If not please suggest an alternative title)**	**Little modification is required in the title. Here with in proposing new title i.e., ''Development of Scoring-Assisted Generative Exploration and Its Applicabilityin designing of enzyme inhibitors''.**	
Is the abstract of the article comprehensive? Do you suggest addition (or deletion) of some points in this section? Please write your suggestions here.	**Abstract is founded in comprehensive manner.No amendments are required.**	
Are subsections and structure of the manuscript appropriate?	**Subsections are organized appropriately, but Figure and Tables to be followed the subsequent paragraphs.**	
Please write few sentences regarding the scientific correctness of this manuscript. Why do think that this manuscript is scientifically robust and technically sound?Minimum 3-4 sentences may be required for this part.	**Technically it sounds good and author has delved in to deeper learning methods and approached well advanced methods.** 1. **In 3.3. QSAR models for target specificity and Single property optimization with SAGE** MAOB is an enzyme that breaks down brain chemicals,(write as catecholamines instead of brain chemicals). 2. **In Results,3.1. Scoring-Assisted Generative Exploration (SAGE), go through following paragraphs to include year of publications** Firstly, I appliedthe SAGE algorithms to general goal-directed benchmarks in GuacaMol[20], with the summarized results in Table 2. For the GuacaMol benchmark, I initializedthe LSTM models using the weights provided by Brown et al. (mention year of publication) Secondly, in myexploration of SAGE's abilities, I paidparticular attention to its performance on the rediscovery and similarity tasks, where the SAGE should generate compounds resembling a specified target molecule removed from the training set. I further validated the ability of SAGE to discover eleven compounds with structurally complex bridged bicyclic rings, which is	

	summarized in Table 3. For the bridged bicyclic ring benchmark, I initialized the LSTM models using the weights provided by Ahn et al. (mention year of publication) 3. Check with page number 29 (Supporting Information for)	
Are the references sufficient and recent? If you have suggestion of additional references, please mention in the review form.	**Number of references are sufficient, whereas, reference numbers 19,30,37 &45 are not having volume/page number.**	
<u>Minor</u> REVISION comments **Is language/English quality of the article suitable for scholarly communications?**	Avoid use of sentences with first person throughout the chapter.Language/Quality of English is good and recommended for scholarly communications.	
Optional/Generalcomments	Overall content and presentation style is good and recommended for further proceedings	

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)*	

Reviewer Details:

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