

Editorial comments:

I reviewed the original manuscript, the reviewer's comments and the revised manuscript. The investigation is scientifically sound and the paper is generally well-written. I have corrected few grammatical errors and style as per enclosed revised manuscript. However, since this work is primarily theoretical in nature and many times the QSAR analyses are not always correct in predicting active compounds for clinical development due to solubility, pharmacokinetics, toxicity, and other related issues, I would like the authors to discuss the limitations of their work in details in a revised manuscript. Also, some of the statistical terms and mathematical equations are not well defined for the average medicinal chemists and pharmacologists who are not actively involved in QSAR analyses, the authors should clarify these terms to make the manuscript understandable to broad segment of pharmaceutical scientists

Author's feedback:

The Editor noticed the relevance of our research to the medicinal chemist and pharmaceutical scientists community around the world. We agree with the editor and thank him for recognizing our efforts. The editor is of the opinion that many times the QSAR analyses are not always correct in predicting active compounds for clinical development due to solubility, pharmacokinetics, toxicity and other related issues and he suggested that the limitations of our work be discussed. We agree with the editor's opinion but since we are aware of the limitations we tried our best in the research to overcome some of these challenges like in the case of training set, we ensured that the training dataset is large enough as such the data we collected reflect the complete property space. Consequently our results can confidently predicted the most likely compounds of the best activity.

The limitations which could not be overcome are hereby discussed in section 2.4 as requested by the editor.

The editor pointed out that some of the statistical terms and equations are not well defined for average medicinal chemist and pharmacologist who are not actively involved in QSAR analyses, on the contrary, the statistical terms and mathematical equation are well defined in section 3.0 to 3.3 with valid references to ease understanding. Attached is the revised manuscript.

Thanks for your cooperation