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| Journal Name: | [**Journal of Pharmaceutical Research International**](https://journaljpri.com/index.php/JPRI) |
| Manuscript Number: | **Ms\_JPRI\_141289** |
| Title of the Manuscript: | **Molecular modeling and virtual screening. Application to computer-aided design of anticancer inhibitors of human dihydroorotate dehydrogenase** |
| Type of the Article | **Research** |

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| PART 1: Comments | | |
|  | Reviewer’s comment **Artificial Intelligence (AI) generated or assisted review comments are strictly prohibited during peer review.** | **Author’s Feedback** (It is mandatory that authors should write his/her feedback here) |
| **Please write a few sentences regarding the importance of this manuscript for the scientific community. A minimum of 3-4 sentences may be required for this part.** | **This topic is important as many researchers are trying to use computer aided drug design tool. There is need to develop anticancer drug. Dihydroorotate dehydrogenase is one of important enzyme for nucleotide synthesis. Molecular docking study can save time and money in drug discovery step.** |  |
| **Is the title of the article suitable?**  **(If not please suggest an alternative title)** | **Computer aided anticancer drug design for human dihydroorotate dehydrogenase inhibitor : Molecular modeling and virtual screening approach** |  |
| Is the abstract of the article comprehensive? Do you suggest the addition (or deletion) of some points in this section? Please write your suggestions here. | 1. **Mathematical equations about free energy should not be included in abstract.** 2. **Abstract should be easy to understand and discuss the outcome of research work.** | Abstract Revised |
| Is the manuscript scientifically, correct? Please write here. | 1. The author had not mentioned about similar molecular docking study for given enzyme. It reflects that literature review is not good.. |  |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.** | <https://www.mdpi.com/1420-3049/27/12/3660>  <https://pubs.acs.org/doi/10.1021/acs.jcim.3c01358>  https://pubmed.ncbi.nlm.nih.gov/24504131/ | Added |
| Is the language/English quality of the article suitable for scholarly communications? | Revision of English language is requested. |  |
| Optional/General comments | **Literature review of recent articles for this topic should be included in this review article.**  **Revise arrangement of figure and tables in the article.** |  |

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| **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)* |  |