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| Book Name: | [Chemical and Materials Sciences: Research Findings](https://www.bookpi.org/bookstore/product/chemical-and-materials-sciences-research-findings-vol-1/)  |
| Manuscript Number: | **Ms\_BPR\_4608** |
| Title of the Manuscript:  | **Study by Molecular Docking of the Interactions between Dihydroorotate Dehydrogenase and a Series of Inhibitors of Pyrrole Derivatives for the treatment of Malaria** |
| Type of the Article | **BOOK CHAPTER** |

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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 *(Please correct the manuscript and highlight that part in the manuscript. 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.** | The enzyme dihydroorotate dehydrogenase (DHODH, PDB ID 6VTN) plays a crucial role in malaria treatment through the pyrimidine biosynthesis pathway, essential for the growth and reproduction of the Plasmodium falciparum parasite. The emergence of drug-resistant parasite strains poses a significant challenge in malaria treatment. Selective inhibition studies of the DHODH enzyme represent novel and distinct approaches compared to traditional targets, aiding in the development of new drugs that can overcome resistance issues, enhance selectivity, and improve clinical efficacy. |  |
| **Is the title of the article suitable?****(If not please suggest an alternative title)** | **Kindly recommend the new title:****Study on the Inhibitory Potential of Pyrrole Derivatives Against Dihydroorotate Dehydrogenase for Malaria Treatment Using Molecular Docking Methods** |  |
| 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. | **Yes, it is.** |  |
| **Is the manuscript scientifically, correct? Please write here.**  | **Yes, it is** |  |
| **Are the references sufficient and recent? If you have suggestions of additional references, please mention them in the review form.****-** | **Please refer to article:**[**https://pubs.acs.org/doi/10.1021/acs.jmedchem.0c00311**](https://pubs.acs.org/doi/10.1021/acs.jmedchem.0c00311)[**https://www.rcsb.org/structure/6vtn**](https://www.rcsb.org/structure/6vtn) |  |
| Is the language/English quality of the article suitable for scholarly communications? | It is acceptable  |  |
| Optional/General comments | If possible, the author should consider adding the following content:1. Analyze the interactions of the receptor PDB ID 6VTN with reference ligands, such as DSM256, DSM502, or some approved and commercialized drugs like Brequinar (DuP-785), to confirm that the pyrrole derivatives studied have similar effects and highlight any differences compared to the reference compounds.
2. Clearly describe the docking methods or algorithms used in the study (e.g., Stepwise Structure, Monte Carlo Sampling, Genetic, Lamarckian Genetic Algorithms, etc.).
3. Describe the method used to determine the active binding site of PDB ID 6VTN.
4. Provide 3D interaction and 3D surface interaction visualizations.
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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)* |  |

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| **Reviewer Details:** |
| Name: | **Pham Van Chung** |
| Department, University & Country | **Vietnam** |