

**Manuscript No.:** Peer J-2022.

**Recommendation:** Minor revision.

**Comments:**

The article entitled “In-silico assay of a dosing vehicle based on chitosan-TiO<sub>2</sub> and modified benzofuran-isatin molecules against *Pseudomonas aeruginosa*” This paper looks scientifically sound, and interesting to the readers of Peer J Physical Chemistry. After addressing the few recommendations made in this article. The manuscript may be accepted for publication in this journal. A few minor corrections are suggested:

1. The abstract is too long; I ask the authors to shorten it and leave only the most important information.
2. Give the proper reason behind the utility of B3LYP/6-31+G(d,p) and M06-2x. A justification must be provided.
3. To put the study in its state of the art, the authors must update the Introduction section, by recent works found in the literature. Introduction section should be revised. Some references which should be added: <https://doi.org/10.1016/j.compbiolchem.2020.107311>, DOI:10.1016/j.saa.2013.11.001, <https://doi.org/10.1016/j.molstruc.2021.131083>, <https://doi.org/10.1016/j.jmrt.2019.11.045>.
4. Why is the choice of the method employed in this study? Proper citation for the used basis set should be introduce.
5. The abbreviations in the manuscript should be provided with the full name before use, e.g "NBO", "DFT", etc.
6. How do the author chose different proteins in molecular docking? Explain more and compare the results found with these found in the literature.
7. The manuscript should be thoroughly scrutinized for punctuations/grammatical errors.

Remark: Accept with minor revision