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Peer Review

Review of: "In Silico Toxicity Assessment of Organophosphates: A DFT and Molecular Docking Study on Their Interaction with Human Serum Albumin (HSA)"

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The article deals with extensive studies on exploring the energetics of various organophosphates with HSA. The results establish the nature of bimolecular interactions as well as the binding stability. However, I need certain clarifications regarding the study:

1. Was BOVINE SERUM ALBUMIN (BSA) involved in the study for comparison with HSA? If carried out, please provide the comparative study.
2. The preferred domain of HSA for which the guest molecules reside is not provided. Further, detailed information on the binding sites, binding domains such as Sudlow binding sites and domains, should be mentioned for each derivative of the organophosphates and should be clearly explained.
3. Were there any unfavourable interactions existing between the host and guest complex?
4. Which forces were predominant in the binding stability of HSA with the organophosphates?
5. Were all the energy parameters, like intermolecular energy, electrostatic, etc., considered in determining the docking score?
6. What is the role of amino acid contribution? Do polar or non-polar amino acids contribute to the stability?
7. Which is the most preferred domain?
8. Certain references regarding the docking of HSA with guest molecules that are published recently are to be added. **Arabian J Chemistry 2023, 16, 5, MAY 2023, 104701, JCIS Open, Volume 12,**

doi.org/10.32388/9YM0GI

December 2023, 100096 https://doi.org/10.1016/j.jciso.2023.100096, Results in Chemistry Vol 11, 2024, 101746, J Saudi Chem Soc., 2021 (25) 101364

A major revision is required for publication; in the present form, it is not suitable.

Declarations

Potential competing interests: No potential competing interests to declare.