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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 presents an in-depth investigation into the energetics of various organophosphates with Human Serum Albumin (HSA). The findings reveal the nature of bimolecular interactions and confirm the binding stability. However, further clarification is needed regarding certain aspects of the study:

1. Was Bovine Serum Albumin (BSA) involved in the study for comparison with Human Serum Albumin (HSA)? If so, please provide details of the comparative study.
2. What is the preferred domain of HSA for guest molecule residence? Please provide detailed information on the binding sites and domains, including Sudlow binding sites, for each derivative of the organophosphates.
3. Were there any unfavorable interactions between the host and guest complex?
4. Which forces predominantly contribute to the binding stability of HSA with the organophosphates?
5. Were all energy parameters, such as intermolecular energy and electrostatic energy, 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 binding domain of HSA for the organophosphates?
8. Certain references regarding the docking of HSA with guest molecules that were published recently are to be added. ***Arabian J Chemistry 2023, 16, 5, MAY 2023, 104701, JCIS Open, Volume 12,***

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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*

9. Addressing these areas thoroughly should help make your study more comprehensive and suitable for publication.

Declarations

Potential competing interests: No potential competing interests to declare.