

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 paper offers a theoretical examination of the possible interactions between OPs and HSA. However, some concerns are worth noting:

1. The introduction is very long compared to the overall word count of the manuscript; it should be summarized and focused more on the objectives of this work, which are studying and understanding the interactions between OPs and HSA. Additionally, the introduction reports some previous experimental studies, which provide context for this paper. Still, it would be better if the authors focused on the in-silico studies and approaches used. The current form of the introduction is more suitable for an experimental-based paper. The introduction should be improved in these regards.
2. The introduction should also mention the originality of this work in the last paragraph.
3. The choice of OPs studied is not clear. What criteria did the authors use for selecting these OPs?
4. In section (3.2. Molecular docking of OP pesticides with HSA protein), the authors describe the results shown in the tables and figures but do not provide further discussion or comparisons with related works. Could the authors explain what underlies the strong binding of Azinphos-methyl compared to other OPs? Could this paper focus solely on the interaction of Azinphos-methyl with HSA, treating the results of the other OPs as preliminary findings? Most of the discussion is centered on Azinphos-methyl, yet the paper is titled "Organophosphates Toxicity."

5. The last reference cited appears in the introduction, which is problematic. The behavior, results, suggested interaction mechanism, and bonding should all be supported by references from the literature. Otherwise, the information provided may lack scientific accuracy.
6. The paper title (In Silico Toxicity Assessment of Organophosphates...) suggests a broader exploration of toxicity. However, this section is brief and only describes results without providing further explanations, discussions, or comparisons.

The current form of the paper is not suitable for publication.

Declarations

Potential competing interests: No potential competing interests to declare.