

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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Reviewer Report on "In Silico Toxicity Assessment of Organophosphates: A DFT and Molecular Docking Study on Their Interaction with Human Serum Albumin (HSA)" by Awadhesh Kumar Verma

Overview:

This manuscript presents a comprehensive in silico analysis of the toxicity of organophosphates (OPs) by investigating their interaction with Human Serum Albumin (HSA) using density functional theory (DFT) and molecular docking techniques. Given the widespread use of OPs and their potential toxicological effects, this study addresses an important and timely research question.

Strengths:

1. Relevance and Importance:

The study addresses a significant and relevant issue by exploring the toxicological effects of OPs, which are widely used as pesticides. The focus on their interaction with HSA provides valuable insights into the molecular mechanisms of their toxicity.

2. Comprehensive Methodology:

The combination of DFT and molecular docking approaches offers a robust framework for analyzing the electronic properties and binding affinities of OPs. This dual approach enhances the reliability and depth of the findings.

3. Detailed Analysis:

The manuscript provides a thorough analysis of key electronic descriptors (HOMO-LUMO gap, electrostatic potential) and their implications for the reactivity of OPs. The molecular docking results are well-explained, highlighting the strong binding affinities and potential interference with HSA's native functions.

4. Molecular Dynamics Simulations:

The inclusion of molecular dynamics simulations adds an additional layer of validation, confirming the stability of the OP-HSA complex over time. This strengthens the overall conclusions drawn from the study.

Weaknesses:

1. In Silico Limitations: While the in silico methods provide valuable predictions, the study would benefit from experimental validation. If possible, including in vitro or in vivo data would strengthen the findings and offer more comprehensive evidence of OP toxicity.

2. Scope of OP Compounds:

The study focuses on a selected set of OP compounds. Expanding the analysis to a broader range of OPs could provide a more comprehensive understanding of their toxicological behavior.

3. Presentation of Results:

Some sections of the manuscript could benefit from clearer presentation. For instance, detailed tables or figures summarizing key findings could enhance the readability and impact of the results.

Recommendations:

1. Experimental Validation:

Consider incorporating experimental data to validate the in silico predictions. This could involve in vitro assays to assess the binding interactions and toxic effects of OPs on HSA.

2. Broader Analysis:

Expand the analysis to include a wider variety of OP compounds. This would provide a more comprehensive assessment of the toxicological risks posed by different OPs.

3. Enhance Clarity:

Improve the clarity and presentation of the results. Detailed visual aids (tables, figures) summarizing key findings could make the manuscript more accessible and impactful.

Conclusion:

Overall, the manuscript presents a valuable and well-conducted study on the toxicity of

organophosphates through their interaction with Human Serum Albumin. The combination of DFT and molecular docking offers a comprehensive and insightful analysis. Addressing the mentioned weaknesses and incorporating the recommendations would further strengthen the manuscript and its contributions to the field.

I hope this structured review helps! If you need any further assistance, feel free to ask.

Thank you, and all the best!

Declarations

Potential competing interests: No potential competing interests to declare.