Qeios

Peer Review

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

Attar Kubaib[1]

1. Chemistry, Thiruvalluvar University, India

This study provided an in-depth look at organophosphates (OPs) using Density Functional Theory (DFT) and molecular docking to explore their toxicity and interaction with Human Serum Albumin (HSA). The research approach was solid, but a few areas could be improved for better clarity and impact:

1. The manuscript tends to repeat details, particularly about the toxic effects of OPs on human health. Consolidating these sections would make the narrative more engaging and easier to follow.
2. Although the study mentions electronic descriptors like the HOMO-LUMO gap, it doesn't fully explain how these properties relate to the toxic effects observed. Providing a clearer connection between these electronic properties and the chemical behavior of OPs would strengthen the analysis.
3. Most figures and tables could benefit from better labeling and more detailed legends. Doing so would make the data more accessible and help readers understand the findings at a glance.

Declarations

Potential competing interests: No potential competing interests to declare.

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