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# Computational Analysis of Dioxin-Like Compounds: Investigating Interactions with AhR and Cytochrome P450 Enzymes

*Monday 9 June 2025 10:45 (15 minutes)*

Dioxin-like compounds (DLCs) are environmental pollutants known for their high toxicity and persistence, primarily exerting their effects through interactions with the aryl hydrocarbon receptor (AhR) and subsequent metabolic processing by cytochrome P450 enzymes. To elucidate the molecular mechanisms underlying these interactions, we employed first-principle computational methods, including density functional theory (DFT) and molecular dynamics (MD) simulations.

Our study focused on analyzing key parameters such as Root Mean Square Deviation (RMSD), Root Mean Square Fluctuation (RMSF), and Solvent Accessible Surface Area (SASA) to assess the conformational stability and dynamics of ligand-AhR complexes. The binding affinities and interaction profiles of various DLCs with AhR were evaluated to identify potential high-affinity ligands.

Furthermore, we investigated the interactions between these ligands and cytochrome P450 enzymes during the metabolic process. By simulating the metabolic pathways, we aimed to predict the biotransformation products and assess their potential toxicities.

Our findings provide insights into the structural and dynamic aspects of DLC interactions with AhR and P450 enzymes, contributing to a better understanding of their toxicological profiles. This computational approach offers a valuable framework for predicting the behavior of environmental toxins and aids in the development of strategies for risk assessment and mitigation.

## Keyword-1

Toxicity assessment

## Keyword-2

Ligand-receptor interactions

## Keyword-3

First-principle study

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