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(G*) (POS-40) First principles study of ligand-protein interaction: A DFT and MD pathway to bioactivity estimation of molecular chemicals

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The aim of this study is to find a pathway to evaluate and predict the bioactivity of molecular chemicals using the first principles approaches. The main question is why molecules with similar structures demonstrate distinct bioactivity properties when interacting with bio-organisms? Addressing this question holds significance not only for applications to environmental safety of chemicals and drug design but also for advancement of our understanding of kinetic process in complex system. The objective is to elucidate such a macroscopic phenomenon through atomic-level physico-chemical properties and ultimately construct a theoretical model capable of delineating the corresponding structure-bioactivity relationships. A directional reactivity pathway has been developed in the first step of study for preliminary estimation of ligand's reactivity with aryl-hydrocarbon receptor (AhR) protein. The general metabolic pathways, specific mechanisms of biochemical transformation, and relevant background knowledge for ligand-protein interactions have been considered. To investigate critical changes stemming from subtle deviations in molecular structures, we utilize two theoretical tools. Specifically, Density Functional Theory (DFT) is used for calculating the electron density distribution and related electric properties, such as dipole moments and localized electrophilicity. Meanwhile, Molecular Dynamic (MD) simulations are applied to investigate and visualize molecular kinetic interactions, emphasizing the influence of steric effects. Theoretical studies on ligand-protein binding orientation, probability, and equilibrium binding positions are conducted and presented as well as their comparison with experimental bioassay results.

Keyword-1

DFT

Keyword-2

Molecular Dynamics

Keyword-3

Toxicity

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