ORGANIC NANOCONE STRUCTURES AS SENSORS FOR METFORMIN DETECTION

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Abstract

In this study, we investigate the interactions between organic nanocone structures and metformin, a widely prescribed drug for managing high blood sugar levels. To gain deeper insights into binding affinities and noncovalent interactions, we employ a multiscale computational approach that integrates various levels of atomistic modeling. Initially, the semiempirical GFN2-xTB method is used to optimize the geometry of these large molecular systems efficiently. Subsequently, selected density functional theory calculations refine the electronic structure properties, focusing on charge distribution and interaction energies. By analyzing electron density topology and noncovalent interaction descriptors, we evaluate the nature, strength, and spatial distribution of intermolecular forces governing metformin adsorption. Additionally, a selected system consisting of a nanocone and a metformin molecule is subjected to molecular dynamics simulations to assess the dynamical properties of the interaction, including stability and binding persistence over time. These findings enhance our understanding of molecular recognition processes at the nanoscale, offering valuable insights for drug delivery, adsorption technologies, and biomedical applications.

Keywords: *adsorption, binding energies, noncovalent interactions, DFT, GFN2-xTB, MD*