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Theoretical and experimental study of anticancer properties of carboxamide ligand

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Abstract

tetrahydrobenzo[d]thiazole-2,6-diyl)dipicolinamide [H2BPT] which was inspired by biological systems synthesized using green chemistry methods in an ionic liquid solvent. The chemical structure of this compound was confirmed using techniques such as ^{1}H-NMR, IR, UV-Vis, and X-Ray. The interaction of this compound with ct-DNA and human serum albumin (HSA) was studied through fluorescence spectroscopy, CD, and UV-Vis. The results indicated that the binding of the compound to the protein was static and led to a reduction in the alpha-helix structure in albumin. Additionally, at low concentrations, it caused DNA structural distortion, indicating therapeutic efficacy at lower doses. Molecular docking simulations and ADMET studies further confirmed and analyzed the interaction between the compound and biological macromolecules.

Key words: carboxamide, human serum albumin, DNA, molecular docking, density functional theory, ADMET

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