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Experimental and Theoretical Approach, Hirshfeld Surface, Reduced Density Gradient, Molecular Docking of a Thiourea Derivative

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Abstract : A thiourea derivative compound was synthesized and subjected to structural analysis using single-crystal X-ray diffraction (XRD). The crystallographic data unveiled its crystallization in the P21/c space group within the monoclinic system. Examination of the dihedral angles indicated a notable non-planar structure. To support and interpret these resulats, density functional theory (DFT) calculations were conducted utilizing the B3LYP functional along with a 6–311 G (d, p) basis set. Additionally, to assess the contribution of intermolecular interactions, Hirshfeld surface analysis and 2D fingerprint plots were employed. Various types of interactions, whether weak intramolecular or intermolecular, within a molecule can significantly impact its stability. The distinctive signature of non-covalent interactions can be detected solely through electron density analysis. The NCI-RDG analysis was employed to investigate both repulsive and attractive van der Waals interactions while also calculating the energies associated with intermolecular interactions and their characteristics. Additionally, a molecular docking study was studied to explain the structure-activity relationship, revealing that the title compound exhibited an affinity energy of -6.8 kcal/mol when docked with B-DNA (1BNA).

Keywords : computational chemistry, density functional theory, crystallography, molecular docking, molecular structure, powder x-ray diffraction, single crystal x-ray diffraction
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