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Crystal Structure, Molecular Docking, Hirshfeld Surfaces and Computational Studies of (2-((1H-Benzo[D]Imidazol-2-Yl) Methoxy)-5-Chlorophenyl)(4-Chlorophenyl)Methanone

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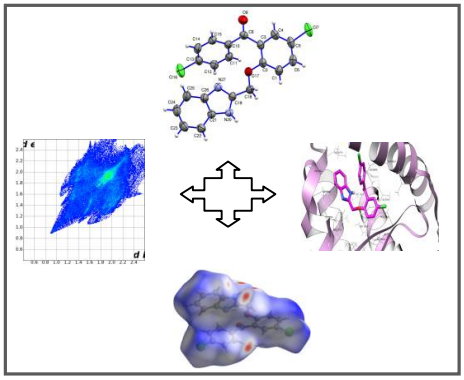
ABSTRACT

The title compound was synthesized and characterized by single crystal X-ray diffraction studies, molecular docking and Hirshfeld surface analysis. The title compound $C_{21}H_{14}N_2O_2Cl_2$ crystallizes in the monoclinic system with the space group of $P2_{1/c}$ with cell parameters a=13.5920(8)Å, b=7.4310(5)Å, c=19.6210(1)Å, β=114.554(6)°, V=1802.6(2)Å^3 and Z=4. The structure exhibited intermolecular interaction of the type C-H...O, molecular docking analysis of the title compound is executed with anti-cancerous target with hER-α protein shown high binding affinity. In addition to this Hirshfeld surface computational analysis were carried out. The major inter-contacts contributing to the Hirshfeld surface are H...H, H...Cl, H...C and H...O.

Graphical Abstract



Keywords: Benzophenone, crystal structure, anticancer, Hirshfeld Surfaces.