



Structural Elucidation and Hirshfeld Surface Analysis of A Novel Piperazine Derivative: (4-Benzhydrylpiperazin-1-Yl)(Morpholino)Methanone

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ABSTRACT

Title compound was prepared from 1-benzhydryl-piperazine and evaluated for antiproliferative activity and structure was characterized using IR, ¹H-NMR, LC-MS spectra and finally the structure was confirmed by X-ray diffraction studies. The compound crystallizes in the monoclinic crystal system with the space group P2₁/c with both the piperazine and the morpholine rings adopting a chair conformation. The structure exhibits both inter and intramolecular hydrogen bonds of the type C--H...O and contributes to the crystal packing. Further, the Hirshfeld surface analysis reveals the nature of intermolecular contacts; the fingerprint plot provides the information about the percentage contribution from the intermolecular contacts to the surface.

Keywords: 1-Benzhydryl-piperazine, carboxamide, antiproliferative activity, Hirshfeld Surface, C--H...O hydrogen bonds.
