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Poster Presentation

Synthesis, X-ray diffraction studies and Hirshfeld surface analysis of (1E)-1-isobutyl-4-(2-(1-pheny

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Imidazo-quinolone have been demonstrated to possess antiviral, antitumor, antiallergic, human toll like reception, and activities. (1E)-1-isobutyl-4-(2-(1immune response modification Imidazo quinolone derivative, phenylethylidene)hydrazinyl)-1H-imidazo[4,5-c] quinolone hydrate (C22H21N5.H2O) was synthesized by condensation of 4hydrazino-1-isobutyl-1H-imidazo[4,5-c]quinolone with acetophenone. The title compound was characterized by FT-IR, NMR spectroscopic techniques and finally the structure was confirmed by X-ray diffraction studies. The structure adopts an E conformation with respect to the C=N bond. The compound exhibits both inter and intramolecular hydrogen bonds of type O-H...N, C-H...O and C-H...N. The intermolecular interaction studies were carried out using Hirshfeld surface analysis. The intermolecular contacts H...H (60%) play a prominent role in the stabilization of crystal and molecular structure of the title molecule. The packing diagram indicates that the molecules exhibit layered stacking and are inter connected by the intermolecular hydrogen bonds.

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Figure: (a) ORTEP diagram of the title molecule with 30% probability. (b) Visualization of intermolecular interactions in the crystal lattice

Keywords: Imidazo-quinolone, Single crystal X-ray diffraction, Hirshfeld surface analysis