



A Significant Approach in which a Carboxylic Acid Group Prevents Bisindole Formation when 2-Formylbenzoic Acid Reacts with Indole: A Crystal Structure Study

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Abstract: Expedite, highly efficient and a novel procedure for the synthesis of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones *via* condensation reaction of indole and 2-formylbenzoic acid catalyzed by glacial acetic acid with excellent yield have been described. The products obtained were characterized by IR, ¹H NMR, LCMS spectral analysis and finally the structure was confirmed by single crystal X-ray diffraction studies. The compound The C₁₆H₁₀FNO₂ crystallizes in the orthorhombic space group Pbc_a with a single molecule in the asymmetric unit. The crystal structure revealed the presence of intermolecular hydrogen bonds of the type N—H...O and C—H...O which contributes to the crystal packing. Further, Hirshfeld surface studies revealed the nature of intermolecular contacts; the importance of the molecular interactions are established from d_{norm} , electrostatic potential and fingerprint plot, which provides the information about the percentage contribution of the individual intermolecular contacts to the surface.

Key Words: Bis-Indoles; 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones; Crystal Structure; Hirshfeld surface analysis, Fingerprint plots.