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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, ^{1}H NMR, LCMS spectral analysis and finally the structure was confirmed by single crystal X-ray diffraction studies. The compound The $C_{16}H_{10}FNO_2$ crystallizes in the orthorthormbic space group Pbca 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...Owhich 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.

Introduction

Indoles are found to be one of the significant groups of compounds used for various physiological and biological activities [1-3]. On the other hand, various bis(indolyl)methanes have also attracted considerable attention due to their potential biological activities [4-7]. Hence while attempting to obtain such lead bioactive bisindolylmethanes we unexpectedly ended with a strange product when we carried out a reaction between 2-formylbenzoic acid and indole in the presence of glacial acetic acid at room temperature stirring for 4-6 hours (**Scheme-1**). Initially one molecule of 2-formylbenzoic acid and two molecules of indole reaction were carried out. But the products obtained was 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones (**4a-b).** Then we realized that the reaction occurred by utilizing mole equivalents of 2-formylbenzoic acid and indole (1:1). Further the same reaction was repeated with mole equivalent of 2-formylbenzoic acid and indole (**Scheme-2**) to furnish the new products **4a** and **4b**.In view of the wide applications associated with the Indole derivatives and in continuation

of our work on new products isolation and their single crystal structure studies [8-11], we report herein an interesting reaction and its end products 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones (**4a-b)**.The product obtained was characterized spectroscopically by NMR and IR techniques and finally the structure was confirmed X-ray diffraction studies.

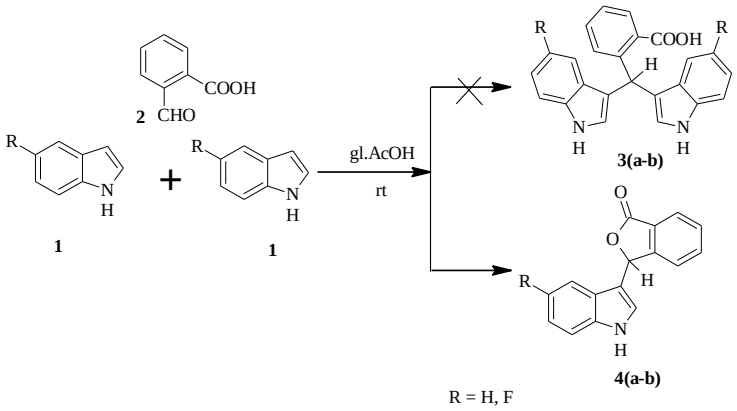
Experimental Procedure

Materials and methods

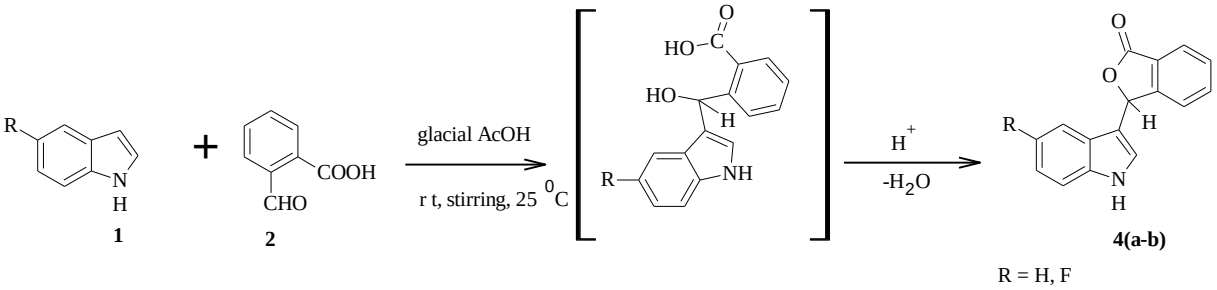
In a flask containing 5 ml of glacial acetic acid and indole (1 mmol, 0.50 g) was added under stirring until all the indole was dissolved. Then 2-formylbenzoic acid (1 mmol, 0.64 g) was added under vigorous stirring. The reaction mixture was allowed to stir for 4-6 h, where the reaction solution turned from light yellow to light pink to dark red color. The product formation was detected by TLC (100 % CH_2Cl_2). After the completion of the reaction, the reaction mixture was added to the ice cold water. The product separated out from the reaction mixture was filtered and washed with water. The crude product was further purified by recrystallization by using methanol furnished white crystals of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4a**) in good yield (80.5%), M.P = 174-176^{0}C. Similarly, the compound 3-(5-fluoro-1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4b**) was also synthesized, purified and recrystallized. (Yield, 83%, and M.P=180-182°C).

Synthesis of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones

The reaction sequence used for synthesis of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4a**) is depicted in **Scheme-1**.The 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4a**) was accomplished by condensation reaction by using commercially available indole (**1**) and 2-formylbenzoic acid (**2**). Stirring the reaction mixture with glacial acetic acid at RT for 4-6 h gave unexpected cyclisation product called 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one(**4a**) instead of corresponding bis(indolyl)methane (**3a**). Thus the resulted crude product was purified by recrystalization using methanol as solvent to get3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4a**). Recrystalization with methanol resulted fine white crystals of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4a**). The product structure was established by single crystal X-ray diffraction studies.

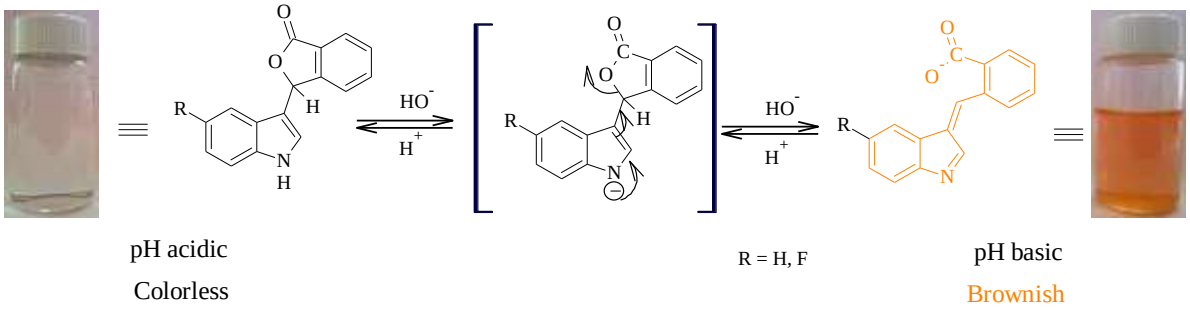


Scheme-1: Reaction of indole (1) and 2-formylbenzoic acid (2) to obtain unexpected 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones (4a-b)



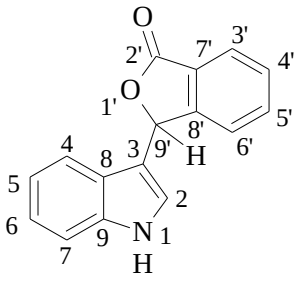
Scheme-2: Mole equivalent reaction of indole (1) and 2-formylbenzoic acid (2) to obtain 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-ones (4a-b)

Similarly, the compound 3-(5-fluoro-1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one **(4b)** was also obtained under the same reaction conditions. Hence, we proved that any structure of appropriate indoles can produce similar products. Since, the structure resembles with the structure of phenolphthalein in its chemical properties, the following reaction with NaOH was checked for compound **4a** and their color change was examined as shown in Scheme-3. Thus we concluded that these compounds can also be very useful in similar application in which phenolphthalein's are being used for biochemical or physico chemical applications.



Scheme-3: Physical changes of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (4a) in both acidic and basic pH

The postulated structure of the newly synthesized 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one compound **4a** was in good agreement with structure based on their IR, ^{1}H NMR, and X-ray diffraction studies.



4a

X-ray Diffraction Studies

A white colored rectangle shaped single crystal of dimensions 0.29×0.26×0.22 mm of the title compound was chosen for an X-ray diffraction study. The X-ray intensity data were collected at a temperature of 296 K on a Bruker Proteum2 CCD diffractometer equipped with an X-ray generator operating at 45 kV and 10 mA, using CuK_α radiation of wavelength 1.54178 Å.Data were collected for 24 frames per set with different settings of φ(0° and 90°), keeping the scan width of 0.5°, exposure time of 2 s, the sample to detector distance of 45.10 mm and 2θvalue at 46.6°. A complete data set was processed using *SAINT PLUS* [12]. The structure was solved by direct methods and refined by full-matrix least squares method on F^2 using *SHELXS* and

SHELXL programs [13]. All the non-hydrogen atoms were revealed in the first difference Fourier map itself.All the hydrogen atoms were positioned geometrically and refined using a riding model with U_{iso}(H) = 1.2 $U_{eq}$and 1.5 U_{eq}(O). After ten cycles of refinement, the final difference Fourier map showed peaks of no chemical significance and the residuals saturated to 0.0343. The geometrical calculations were carried out using the program *PLATON* [14].The molecular and packing diagrams were generated using the software *MERCURY* [15].

Hirshfeld surface calculations

Hirshfeld surface analysis was carried out and finger print plots were plotted using the software Crystal Explorer 3.0 [16]. The d_{norm} plots were mapped with color scale in between −0.18 au (blue) and 1.4 au (red). The 2D fingerprint plots [17, 18] were displayed by using the expanded 0.6–2.8 Å view with the d_e and d_i distance scales displayed on the graph axes. When the cif file was uploaded into the Crystal Explorer software, all bond lengths to hydrogen were automatically modified to typical standard neutron values i.e., C–H = 1.083Å.

Results and discussion

The compound **4a** exhibited IR absorption band at 3311 cm^{-1}due to indole -NH group, band at 3055 cm^{-1} indicates -CH- stretching, another characteristic absorption band at 1732 cm^{-1} which is slightly higher stretching frequency (C=O) strongly suggest the presence of cyclic ester group in compound **4a (Figure 2).**

The ^{1}H NMR spectra (**Figure 1(a) and 1(b)**) of the compound 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (**4a**) showed the 10 aromatic protons between 6.76-8.36 ppm. In this, one sharp singlet at δ=6.96 signifies the presence of tertiary proton which is located at the junction of the indole ring and benzo-2-furanone rings linked together. Further a broad singlet of indole -NH appears at 11.31 ppm, and remaining aromatic protons appears as triplet at δ=6.87 ppm with coupling constant, J=7.00 Hz, another in the range of 7.08 ppm with coupling constant, *J*=7.60 Hz, at 7.40 ppm with coupling constant, *J*=8.40 Hz, the four doublet, one in the δ=6.78 ppm with coupling constant, *J*=8.00 Hz, at 7.40 ppm with coupling constant *J*=8.40 Hz, at 7.95ppm with coupling constant, *J*=7.60 Hz respectively are in consistence with the depicted structure.

Thus from all these spectral evidence and single crystal structural analysis the structure of compound **4a** was confirmed.

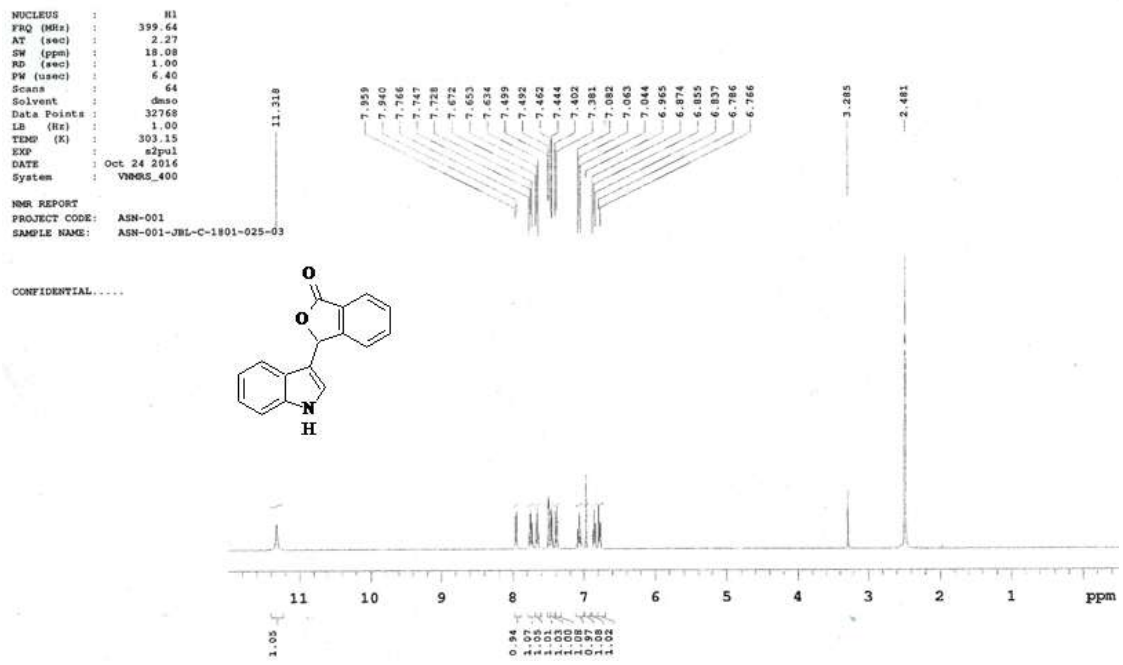


Figure 1(a): ^{1}H NMR Spectrum of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (4a)

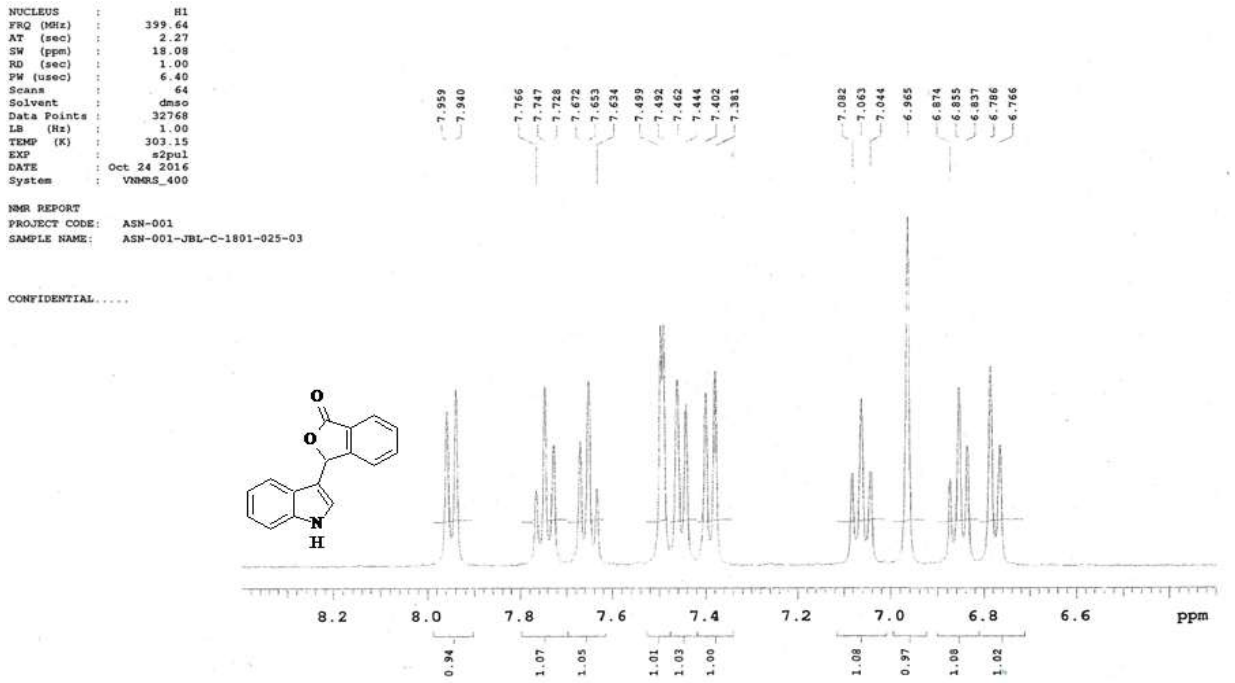


Figure 1(b): ^{1}H NMR Spectrum of 3-(1*H*-indol-3- yl)-2-benzofuran-1(3*H*)-one (4a)

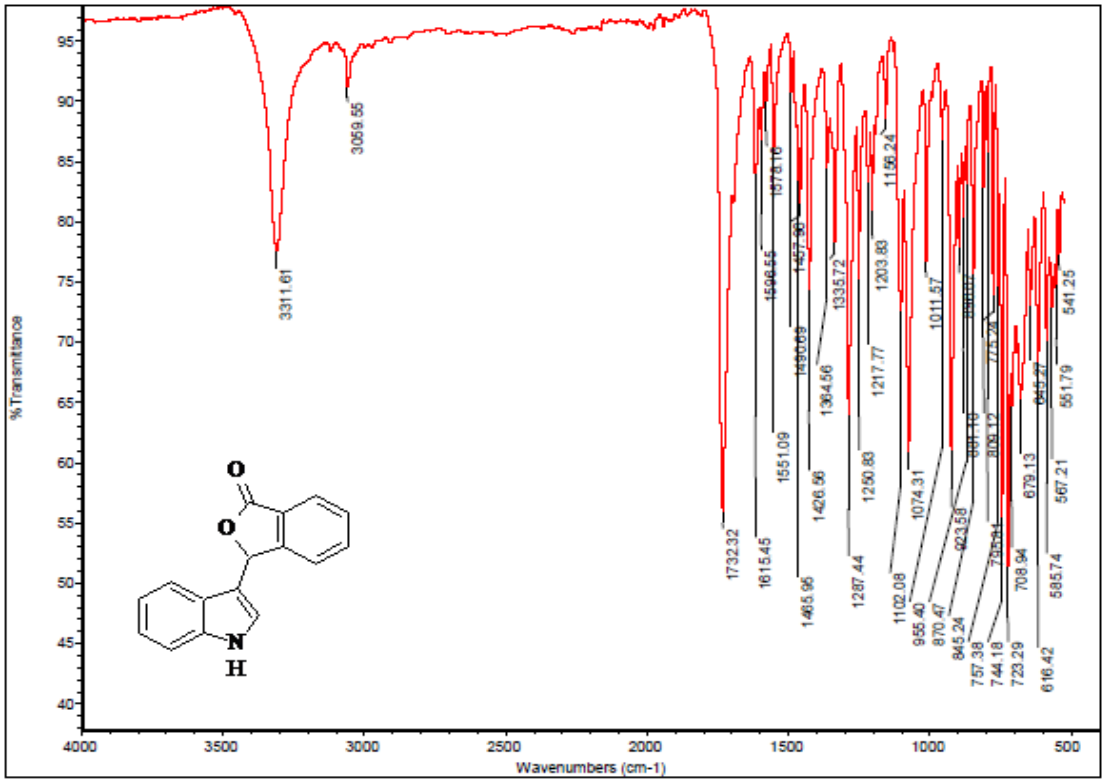


Figure 2: IR Spectrum of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (4a)

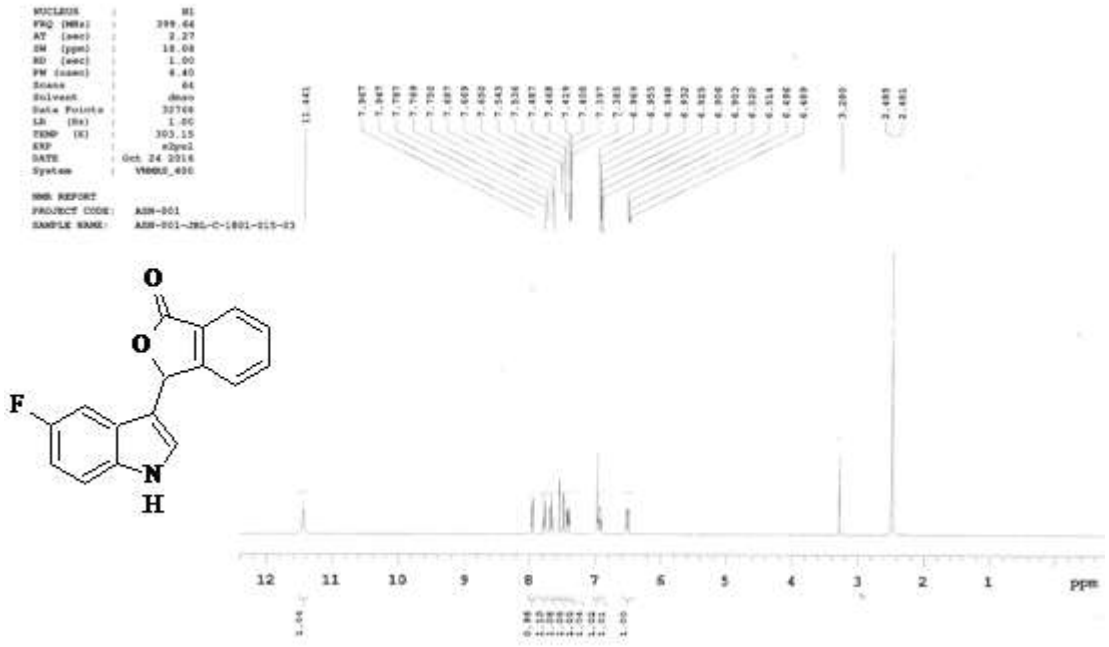


Figure 3(a):^{1}H NMR Spectrum of 3-(5-fluoro-1H-indol-3-yl)-2-benzofuran-1(3H)-one (4b)

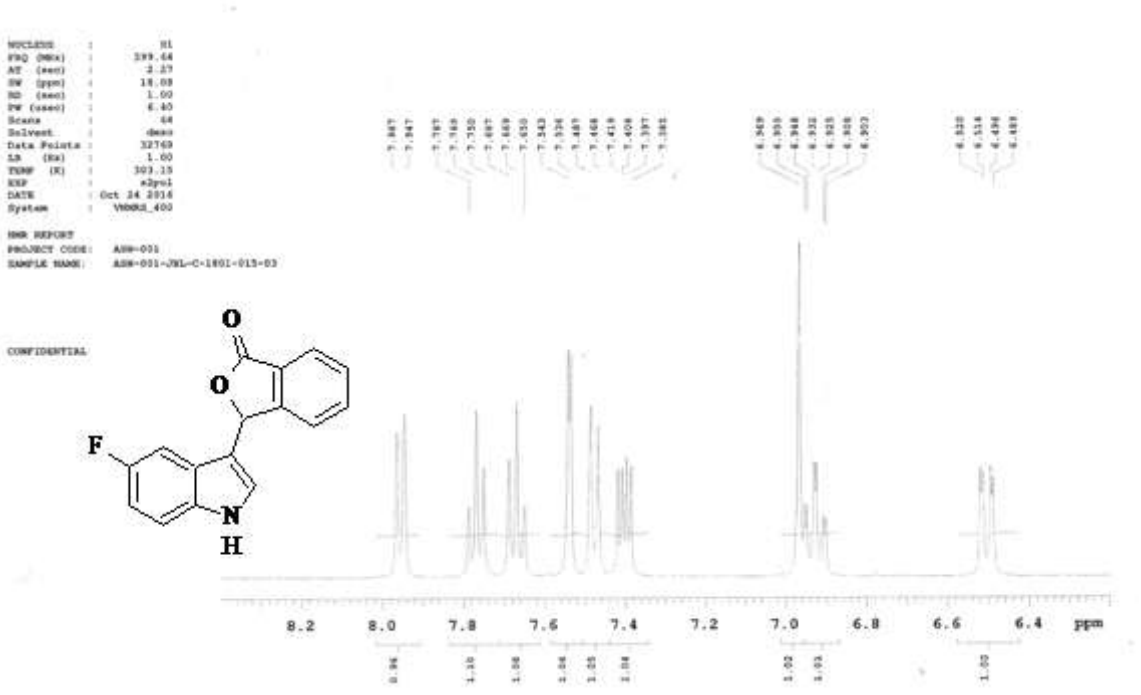


Figure 3(b):^{1}H NMR Spectrum of 3-(5-fluoro-1H-indol-3-yl)-2-benzofuran-1(3H)-one (4b).

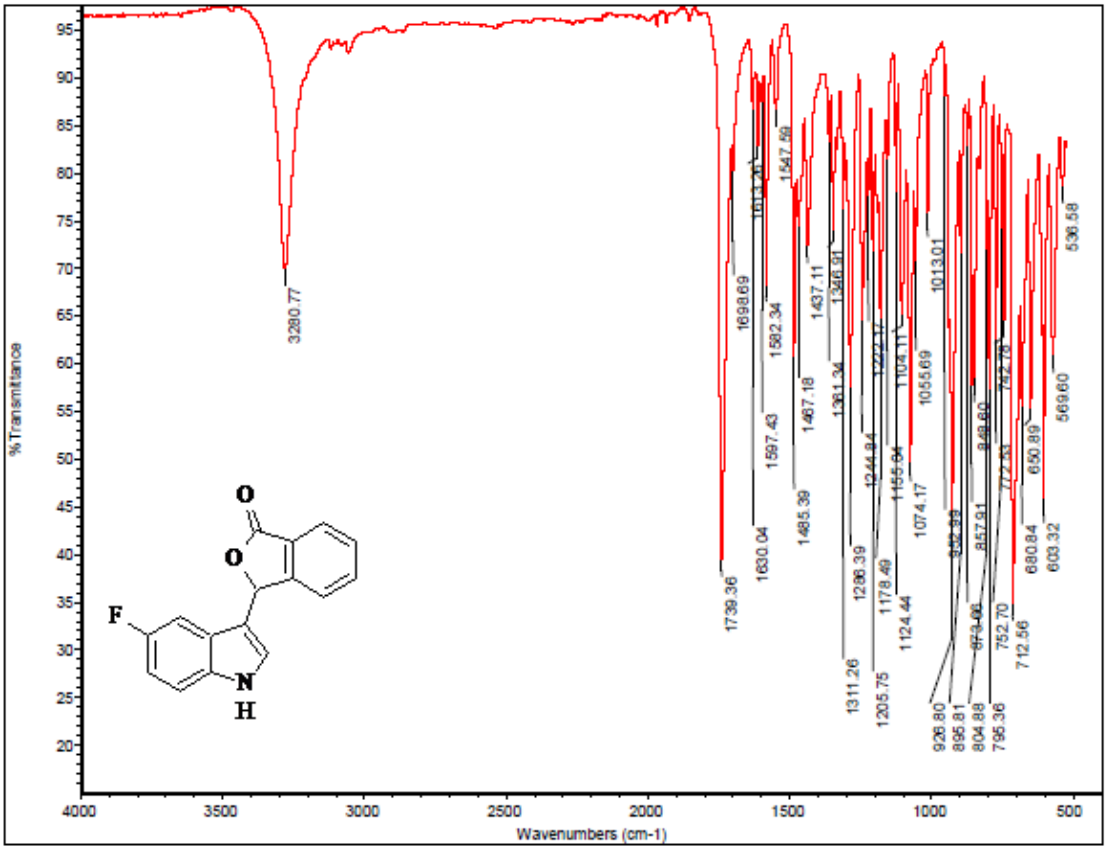


Figure 4: IR Spectrum of 3-(5-fluoro-1H-indol-3-yl)-2-benzofuran-1(3H)-one (4b).

Spectral data of 3-(1*H*-indol-3-yl)-2-benzofuran-1(3*H*)-one (4a)

IR (KBr) (v_{max}/cm^{-1}): 3311 (N-H), 3055 (C-H), 1732 (C=O), 1615 (C-C), 1287 (C-N), 1073(=C-H). ^{1}H NMR (400 MHz, DMSO): δ=6.786 (d, *J* = 8.00 Hz, 1H), 6.874 (t, *J*=7.00 Hz, 1H), 6.965 (s, 1H), 7.082 (t, *J*=7.6 Hz, 1H), 7.402 (d, *J*=8.4 Hz, 1H), 7.462 (d, *J*=7.2 1 H), 7.499(s. 1H). 7.672 (t, *J*=7.6 Hz, 1H), 7.766 (t, *J*=7.6 Hz, 1H), 7.959 (d, *J*=7.60 Hz, 1H), 11.31 (s, 1H) ppm.

Spectral data of 3-(5-fluoro-1H-indol-3-yl)-2-benzofuran-1(3H)-one (4b)

IR (KBr) (v_{max}/cm^{-1}): 3280 (N-H), 3055 (C-H), 1739 (C=O), 1311 (C-N), 1074(=C-H). ^{1}H NMR (400 MHz, DMSO): δ=6.520 (d, *J*=2.4 Hz, 1H), 6.955 (d, *J*=5.6 Hz, 1H), 6.969 (s. 1H). 7.397 (t, *J* = 4.8 Hz, 1H), 7.419 (d, *J*=4.4 Hz, 1H), 7.487(s, 1H), 7.669 (t, *J*=7.6 Hz, 1H), 7.787 (t, *J*=7.2 Hz, 1H), 7.967 (d, *J*=8 Hz, 1H), 11.441 (s, 1H) ppm.

Crystal structure analysis

The molecular structure of the title compound $C_{16}H_{10}FNO_2$ has been confirmed by single crystal X-ray diffraction analysis, which revealed that the compound crystallizes in theorthorhombic space group *Pbca*with unit cell parameters *a* =16.5775(4) Å, *b* = 7.5072(2)Å, *c* = 20.1067(5)Å, *α* = *β* = γ = 90.00^o, *Z* = 8, *V* = 2502.29(11)Å^3. The ORTEP of the molecule with displacement ellipsoids drawn at 50 % probability level is shown in **Figure 5**. The crystal data and the structure refinement details are given in **Table 1.** The molecule is non-planar whereas both the fluoro-indole and the benzopyran rings are planar with the atoms C2 and C11 deviating 0.023(1) Å and 0.035(1) Å from their mean planes respectively. The dihedral angle between the two fused ring planes is 85.15(4)° indicating that they are nearly orthogonal to each other. The structure exhibits intermolecular hydrogen bonds of the type N—H...O and C—H...O. The hydrogen bond N1—H1...O20 has a length of 2.7921(16) Å and an angle of 153° whereas the other hydrogen bond C11—H11...O12 has a length of 3.3238(16) Å and an angle of 154° with symmetry codes *-1/2+x,y,3/2-z* and *1-x,1/2+y,3/2-z* respectively.

These hydrogen bonds links the molecules to chains and the molecules exhibit layered stacking when viewed down along the *b* axis (**Figure 6**).

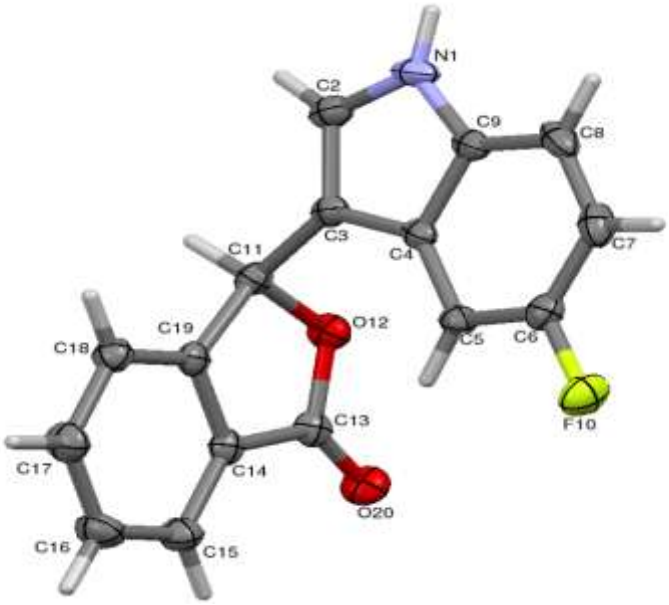


Figure 5: ORTEP of the molecule with thermal ellipsoids drawn at 50% probability.

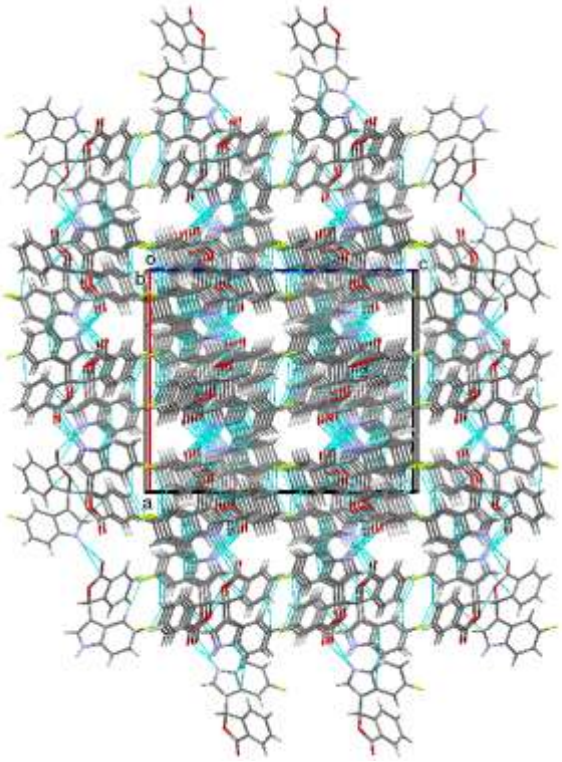


Figure 6: Packing of the molecules when viewed down along the *b* axis. The dotted line represents hydrogen bond interactions.

Table 1: Crystal data and structure refinement details

Parameter	value
CCDC deposit No.	CCDC 1511459
Empirical formula	$C_{16}H_{10}FNO_2$
Formula weight	267.25

Temperature	296 (2) K
Wavelength	1.54178 Å
Crystal system, space group	Orthorhombic, *Pbca*
Unit cell dimensions	a = 16.5775(4) Å b = 7.5072(2) Å c = 20.1067(5) Å $\alpha = \beta = \gamma$ =90.00°
Volume	2502.29(11) Å^3
Z	8
Density(calculated)	1.419 Mg m $^{-3}$
Absorption coefficient	0.871 mm $^{-1}$
F_{000}	1104
Crystal size	0.29 × 0.26 × 0.22 mm
θ range for data collection	4.40° to 64.71°
Index ranges	$-10 \leq h \leq 12$ $-6 \leq k \leq 8$ $-23 \leq l \leq 20$
Reflections collected	12616
Independent reflections	2068 [R int = 0.0335]
Absorption correction	multi-scan
Refinement method	Full matrix least-squares on F ^{2}
Data / restraints / parameters	2068 / 0 / 181
Goodness-of-fit on F^2	1.122
Final [I > 2σ(I)]	*R1* = 0.0343,, *wR2* = 0.0978
R indices (all data)	*R1* = 0.0354, *wR2* = 0.0989
Largest diff. peak and hole	0.169 and −0.210 e Å $^{-3}$

Table 2: Bond lengths (Å)

Atoms	Length	Atoms	Length
C4-C5	1.406(2)	C11-O12	1.485(2)
C4-C9	1.415(2)	C11-C19	1.505(2)
C4-C3	1.437(2)	O12-C13	1.357(2)
N1-C2	1.359(2)	C13-O20	1.212(2)
N1-C9	1.377(2)	C13-C14	1.465(2)
C2-C3	1.369(2)	C14-C19	1.382(2)
C3-C11	1.482(2)	C14-C15	1.386(2)
C5-C6	1.366(2)	C15-C16	1.381(2)
C6-F10	1.370(2)	C16-C17	1.395(2)
C6-C7	1.394(2)	C17-C18	1.388(2)
C7-C8	1.379(2)	C18-C19	1.388(2)
C8-C9	1.393(2)		

Table 3: Bond angles (°)

Atoms	Angles	Atoms	Angles
C5-C4-C9	119.02(13)	C3-C11-O12	109.91(11)
C5-C4-C3	134.31(12)	C3-C11-C19	117.06(11)
C9-C4-C3	106.64(12)	O12-C11-C19	102.85(10)
C2-N1-C9	109.22(11)	C13-O12-C11	110.74(10)
N1-C2-C3	110.32(13)	O20-C13-O12	121.51(12)

C2-C3-C4	106.41(12)	O20-C13-C14	129.71(13)
C2-C3-C11	125.53(13)	O12-C13-C14	108.78(11)
C4-C3-C11	128.03(12)	C19-C14-C15	122.50(13)
C6-C5-C4	116.92(13)	C19-C14-C13	108.34(12)
C5-C6-F10	118.10(13)	C15-C14-C13	129.16(12)
C5-C6-C7	124.59(14)	C16-C15-C14	117.04(13)
F10-C6-C7	117.31(12)	C15-C16-C17	120.96(14)
C8-C7-C6	119.18(14)	C18-C17-C16	121.56(14)
C7-C8-C9	117.93(13)	C19-C18-C17	117.43(13)
N1-C9-C8	130.21(13)	C14-C19-C18	120.50(13)
N1-C9-C4	107.41(12)	C14-C19-C11	109.23(11)
C8-C9-C4	122.35(13)	C18-C19-C11	130.25(12)

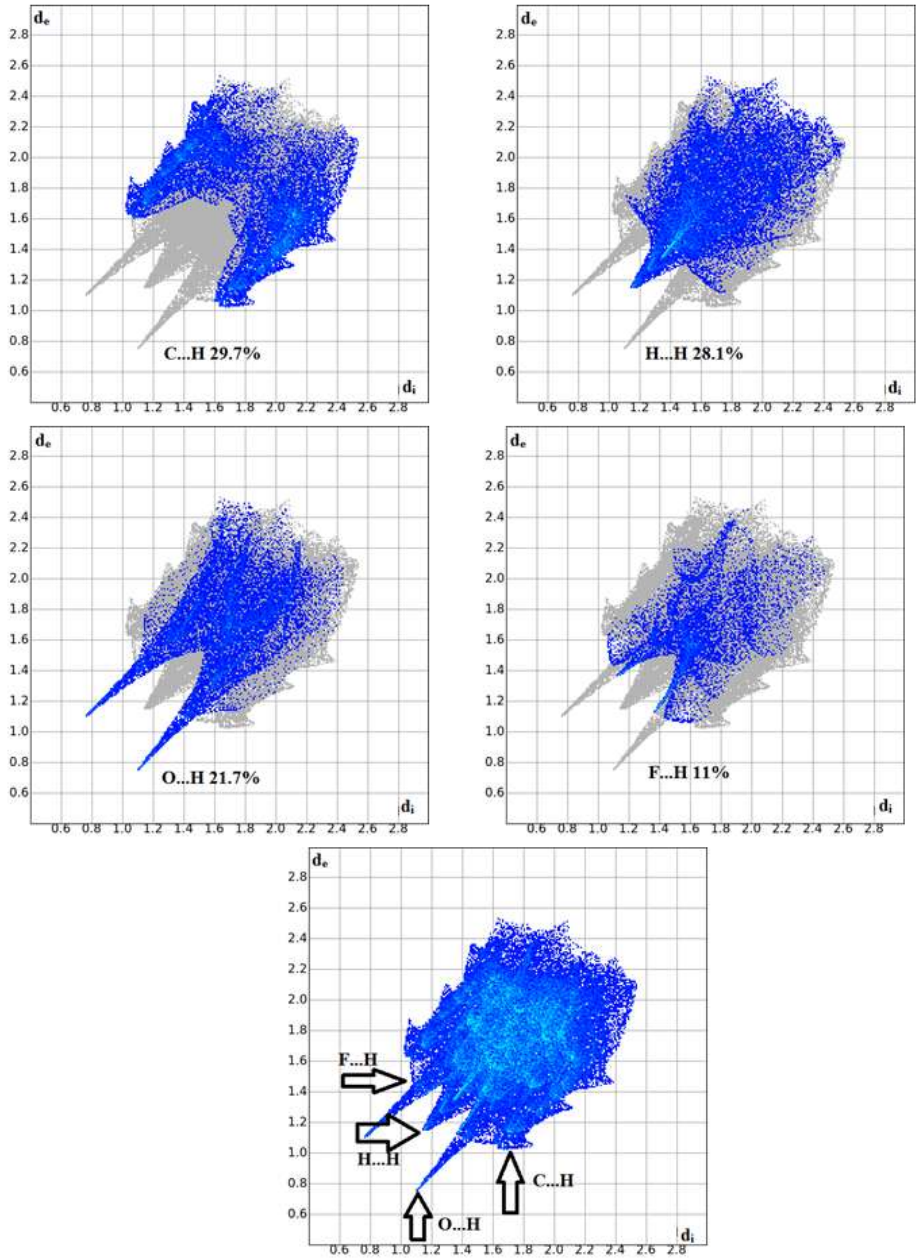


Figure 7: Fingerprint plots of the title compound showing H···H, C···H, O···H and F···H interactions. Here d_i is the closest internal distance from a given point on the Hirshfeld surface and d_e is the closest external contacts.

Hirshfeld surface analysis is an effective tool for exploring packing modes and intermolecular interactions in molecular crystals, as they provide a visual picture of intermolecular interactions and of molecular shapes in a crystalline environment. Surface features characteristic of different types of intermolecular interactions can be identified, and these features can be revealed by color coding distances from the surface to the nearest atom exterior (d_e plots) or interior (d_i plots) to the surface. This gives a visual picture of different types of interactions present and also reflects their relative contributions from molecule to molecule. Further, 2D fingerprint plots (FP), in particular the breakdown of FP into specific atom…atom contacts in a crystal, provide a quantitative idea of the types of intermolecular contacts experienced by molecules in the bulk and presents this information in a convenient colour plot. Hirshfeld surfaces comprising d_{norm} surface and Fingerprint plots were generated and analysed for the title compound in order to explore the packing modes and intermolecular interactions. The two dimensional fingerprint plots from Hirshfeld surface analyses **Figure 7**, illustrates the difference between the intermolecular interaction patterns and the relative contributions to the Hirshfeld surface (in percentage) for the major intermolecular contacts associated with the title compound. Importantly, C...H (29.7%) bonding appears to be a major contributor in the crystal packing, whereas the H...H (28.1%), O...H (21.7%), F...H(11%) plots also reveal the information regarding the intermolecular hydrogen bonds thus supporting for N—H...O and C—H...O intermolecular interactions. This intermolecular contact is highlighted by conventional mapping of d_{norm} and electrostatic potential on molecular Hirshfeld surfaces as shown in **Figure 8**. The red spots over the surface indicate the intercontacts involved in hydrogen bond. The dark-red spots on the d_{norm} surface arise as a result of the short interatomic contacts, i.e., strong hydrogen bonds, while the other intermolecular interactions appear as light-red spots.

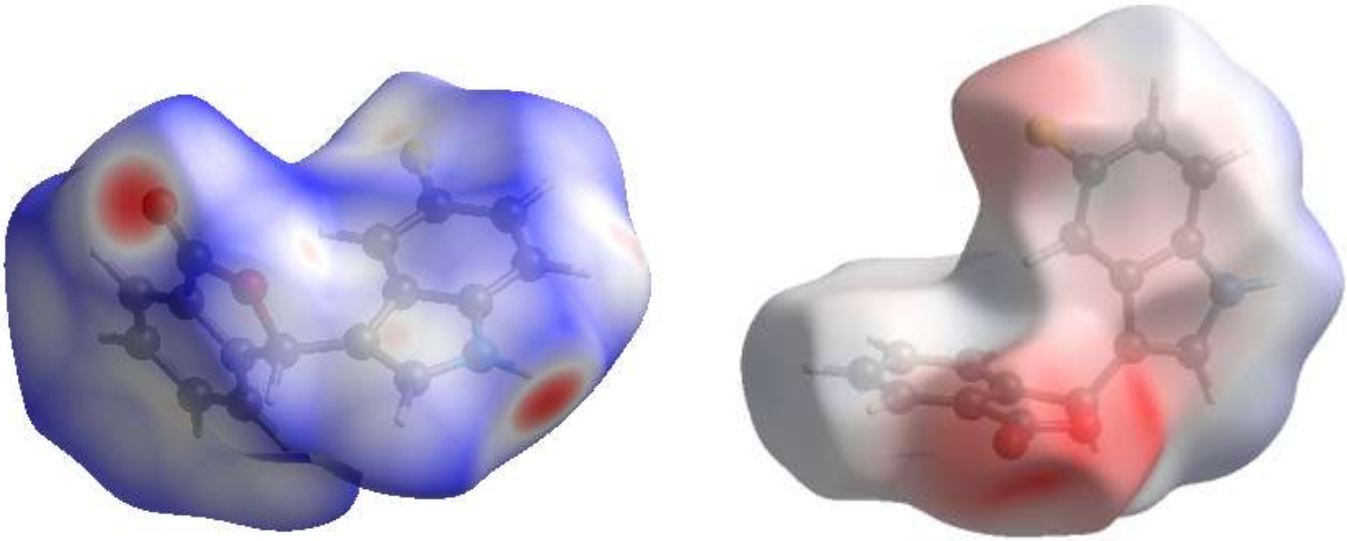


Figure 8: d_{norm} and electrostatic potential mapped on Hirshfeld surface for visualizing the intermolecular contacts

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