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5-(2-Hydroxybenzoyl)-2-(1*H*-indol-3-yl)pyridine-3-carbonitrile

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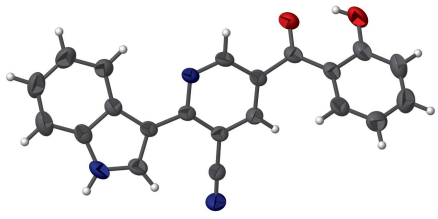
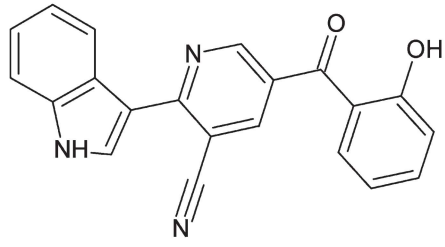
In the title compound, $C_{21}H_{13}N_3O_2$, the indole and pyridine rings are planar. The pyridine ring is in an antiperiplanar (−*ap*) orientation with the indole ring system and an antiperiplanar (+*ap*) orientation with the hydroxyphenyl ring. An intramolecular O—H···O hydrogen bond stabilizes the molecular structure. In the crystal, N—H···N hydrogen bonds involving the indole NH group and the cyanide nitrogen atom lead to the formation of a two-dimensional supramolecular network lying parallel to (011).

3D view



Chemical scheme



Structure description

Indole ring systems have become an important structural component in many pharmaceutical agents (Sundberg, 1996). Substituted indoles have been refered to as privileged structures since they are capable of binding to many receptors with high affinity (Evans *et al.*, 1988). Some indole derivatives possess cytotoxic activity (Muratake *et al.*, 1994). Indole and its bioisosters and derivatives have antimicrobial activity against Gram-negative and Gram-positive bacteria, the yeast *Candida albicans* and *Enterobacter*, *Pseudomonas aeruginosa*, *E. coli*, and *Staphylococcus epidermidis* (Biswal *et al.*, 2012).

The structure of the title compound is shown in Fig. 1. The C—N distances range from 1.345 (2) to 1.370 (2) Å, and are in good agreement with the related reported values (Vishnupriya *et al.*, 2014). The C14—O1 and C21—N3 bond lengths are 1.2347 (14) Å and 1.1413 (16) Å, respectively, in agreement with values reported by Vimala *et al.* (2015), confirming the presence of double and triple bonds. The pyridine ring (C9/N2/C10–C13) is in an antiperiplanar (−*ap*) orientation with the indole ring system (C1/N1/C2–C8) and in an antiperiplanar (+*ap*) orientation with the hydroxyphenyl ring (C15–C20), as evidenced by the torsion angles C7—C8—C9—C13 = −163.54 (11)° and C10—

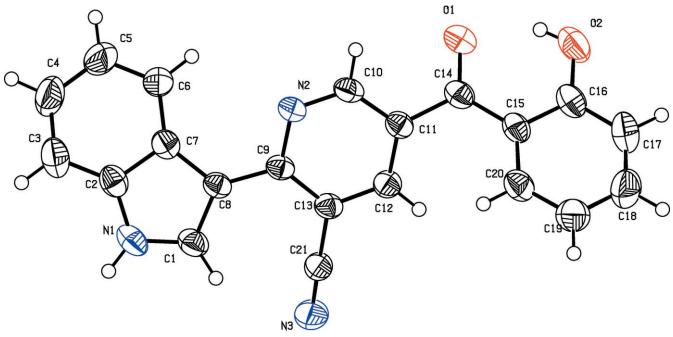


Figure 1
The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level.

C11—C14—C15 = 155.15 (11)°, respectively. An intramolecular O—H···O hydrogen bond (Table 1) stabilizes the molecular structure.

In the crystal, N—H···N hydrogen bonds (Table 1) between the indole NH group and the cyanide nitrogen atom result in a two-dimensional supramolecular network lying parallel to (011) (Fig. 2).

Synthesis and crystallization

A mixture of 3-formylchromone (1 mmol), cyanoacetylindole (1 mmol) and ammonium acetate (1 mmol) in DMF and a catalytic amount of $SnCl_2·2H_2O$ (0.020 mol%) was added and refluxed for about 3 h. After completion of the reaction, the solvent was removed under reduced pressure and the residue was purified by column chromatography on siliga gel (3:97% ethyl acetate and petetroleum ether) to afford pure product in 94% yield. The purified compound was recrystallized from ethanol through slow evaporation of the solvent.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

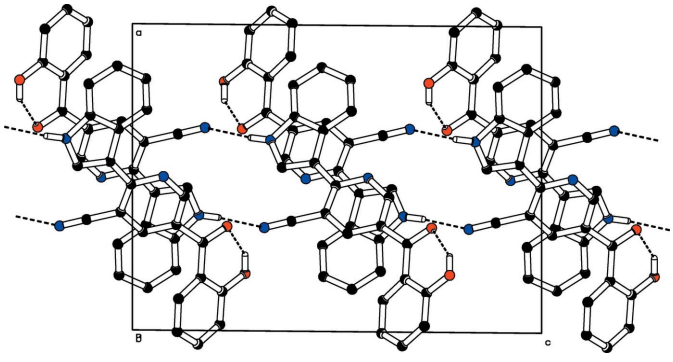


Figure 2
The packing of the molecules in the crystal structure. The dashed lines indicate hydrogen bonds.

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N3^{i}	0.86	2.15	3.0016 (17)	171
O2—H2···O1	0.82	1.84	2.5653 (14)	146

Symmetry code: (i) $-x+1, y+\frac{1}{2}, -z-\frac{1}{2}$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{13}N_3O_2$
M_r	339.34
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, b, c (Å)	12.4764 (6), 7.8471 (3), 16.7265 (8)
β (°)	90.478 (2)
V (Å^3)	1637.53 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.35 × 0.28 × 0.15
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2008)
T_{min}, T_{max}	0.969, 0.986
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10911, 4105, 2665
R_{int}	0.019
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.669
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.121, 1.57
No. of reflections	4105
No. of parameters	237
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.17

Computer programs: *APEX2* and *SAINT* (Bruker, 2008), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *ORTEP-3 for Windows* (Farrugia, 2012).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{21}H_{13}N_3O_2$
M_r = 339.34
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 12.4764 (6) Å
b = 7.8471 (3) Å
c = 16.7265 (8) Å
β = 90.478 (2)°
V = 1637.53 (13) Å^3
Z = 4
$F(000)$ = 704
D_x = 1.377 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2665 reflections
θ = 1.6–28.4°
μ = 0.09 mm^{-1}
T = 298 K
Block, colorless
0.35 × 0.28 × 0.15 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2008)
T_{min} = 0.969, T_{max} = 0.986
10911 measured reflections
4105 independent reflections
2665 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 28.4°, θ_{min} = 1.6°
h = −16→13
k = −10→9
l = −22→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.121
S = 1.57
4105 reflections
237 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0486P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.020
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0087 (17)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.53477 (11)	0.87467 (16)	−0.13362 (8)	0.0454 (3)
H1	0.4722	0.8559	−0.1629	0.054*
C2	0.69959 (10)	0.96028 (15)	−0.10314 (8)	0.0443 (3)
C3	0.80237 (11)	1.02854 (18)	−0.10597 (10)	0.0611 (4)
H3	0.8296	1.0746	−0.1528	0.073*
C4	0.86139 (12)	1.0249 (2)	−0.03697 (12)	0.0765 (5)
H4	0.9300	1.0710	−0.0364	0.092*
C5	0.82078 (12)	0.9534 (2)	0.03258 (11)	0.0775 (6)
H5	0.8632	0.9525	0.0786	0.093*
C6	0.71998 (10)	0.88427 (19)	0.03513 (9)	0.0574 (4)
H6	0.6944	0.8362	0.0821	0.069*
C7	0.65674 (10)	0.88730 (15)	−0.03363 (8)	0.0407 (3)
C8	0.54967 (9)	0.82906 (14)	−0.05491 (7)	0.0364 (3)
C9	0.47648 (9)	0.74161 (13)	−0.00264 (7)	0.0345 (3)
C10	0.43851 (9)	0.66464 (15)	0.12686 (7)	0.0409 (3)
H10	0.4578	0.6690	0.1807	0.049*
C11	0.34536 (9)	0.57542 (15)	0.10706 (7)	0.0376 (3)
C12	0.32069 (9)	0.56672 (15)	0.02623 (7)	0.0392 (3)
H12	0.2611	0.5054	0.0089	0.047*
C13	0.38481 (9)	0.64939 (14)	−0.02888 (7)	0.0364 (3)
C14	0.28746 (11)	0.48524 (15)	0.17204 (8)	0.0430 (3)
C15	0.17239 (10)	0.44727 (16)	0.16690 (7)	0.0424 (3)
C16	0.12797 (11)	0.32598 (17)	0.21906 (9)	0.0510 (4)
C17	0.02012 (12)	0.2849 (2)	0.21349 (10)	0.0673 (5)
H17	−0.0082	0.2017	0.2468	0.081*
C18	−0.04463 (13)	0.3656 (2)	0.15956 (11)	0.0717 (5)
H18	−0.1169	0.3368	0.1564	0.086*
C19	−0.00423 (11)	0.4898 (2)	0.10947 (9)	0.0632 (4)
H19	−0.0493	0.5464	0.0738	0.076*
C20	0.10269 (11)	0.52865 (18)	0.11289 (8)	0.0498 (4)
H20	0.1298	0.6110	0.0786	0.060*
C21	0.35909 (10)	0.62929 (17)	−0.11168 (8)	0.0438 (3)
N1	0.62325 (9)	0.95015 (13)	−0.16227 (6)	0.0499 (3)
H1A	0.6308	0.9865	−0.2104	0.060*
N2	0.50172 (8)	0.74344 (12)	0.07581 (6)	0.0392 (3)

N3	0.33755 (10)	0.60956 (18)	−0.17749 (7)	0.0645 (4)
O1	0.34049 (8)	0.44114 (13)	0.23117 (6)	0.0621 (3)
O2	0.18699 (9)	0.24606 (14)	0.27537 (7)	0.0697 (3)
H2	0.2482	0.2840	0.2753	0.105*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0571 (8)	0.0470 (7)	0.0320 (8)	−0.0046 (6)	0.0009 (6)	−0.0008 (5)
C2	0.0465 (8)	0.0416 (7)	0.0451 (9)	0.0062 (5)	0.0104 (6)	0.0042 (5)
C3	0.0499 (9)	0.0560 (9)	0.0778 (12)	0.0058 (6)	0.0199 (8)	0.0196 (7)
C4	0.0375 (8)	0.0842 (12)	0.1078 (15)	−0.0035 (7)	−0.0015 (9)	0.0368 (10)
C5	0.0478 (9)	0.0969 (12)	0.0875 (14)	−0.0088 (8)	−0.0205 (9)	0.0371 (10)
C6	0.0441 (8)	0.0715 (9)	0.0564 (10)	−0.0035 (6)	−0.0074 (7)	0.0228 (7)
C7	0.0402 (7)	0.0400 (6)	0.0419 (8)	0.0065 (5)	0.0047 (6)	0.0050 (5)
C8	0.0402 (7)	0.0386 (6)	0.0305 (7)	0.0043 (5)	0.0017 (5)	−0.0006 (5)
C9	0.0381 (6)	0.0364 (6)	0.0291 (7)	0.0063 (5)	0.0006 (5)	−0.0018 (5)
C10	0.0465 (7)	0.0479 (7)	0.0282 (7)	0.0030 (5)	−0.0016 (6)	0.0013 (5)
C11	0.0410 (7)	0.0396 (6)	0.0324 (7)	0.0033 (5)	0.0039 (5)	−0.0006 (5)
C12	0.0397 (7)	0.0429 (6)	0.0349 (8)	−0.0001 (5)	0.0019 (6)	−0.0058 (5)
C13	0.0383 (7)	0.0421 (6)	0.0289 (7)	0.0044 (5)	0.0014 (5)	−0.0046 (5)
C14	0.0524 (8)	0.0439 (7)	0.0327 (8)	0.0001 (5)	0.0032 (6)	−0.0010 (5)
C15	0.0483 (7)	0.0458 (7)	0.0332 (8)	−0.0002 (5)	0.0100 (6)	−0.0021 (5)
C16	0.0582 (9)	0.0535 (7)	0.0415 (9)	0.0012 (6)	0.0142 (7)	0.0014 (6)
C17	0.0595 (10)	0.0708 (10)	0.0719 (13)	−0.0104 (7)	0.0225 (9)	0.0100 (8)
C18	0.0482 (9)	0.0942 (13)	0.0730 (13)	−0.0084 (8)	0.0133 (9)	−0.0017 (10)
C19	0.0504 (9)	0.0874 (11)	0.0521 (10)	0.0078 (8)	0.0042 (7)	0.0025 (8)
C20	0.0529 (8)	0.0564 (8)	0.0403 (8)	0.0034 (6)	0.0101 (6)	0.0018 (6)
C21	0.0402 (7)	0.0572 (8)	0.0342 (8)	−0.0042 (5)	0.0034 (6)	−0.0070 (6)
N1	0.0678 (8)	0.0498 (6)	0.0323 (7)	−0.0033 (5)	0.0102 (6)	0.0029 (5)
N2	0.0430 (6)	0.0465 (6)	0.0282 (6)	−0.0023 (4)	−0.0006 (5)	0.0015 (4)
N3	0.0605 (8)	0.0974 (10)	0.0357 (8)	−0.0149 (7)	−0.0007 (6)	−0.0136 (6)
O1	0.0644 (6)	0.0780 (7)	0.0438 (6)	−0.0103 (5)	−0.0053 (5)	0.0185 (5)
O2	0.0717 (7)	0.0794 (7)	0.0583 (8)	−0.0027 (6)	0.0100 (6)	0.0290 (6)

Geometric parameters (Å, º)

C1—N1	1.3446 (17)	C11—C12	1.3857 (16)
C1—C8	1.3754 (17)	C11—C14	1.4891 (18)
C1—H1	0.9300	C12—C13	1.3867 (17)
C2—N1	1.3697 (16)	C12—H12	0.9300
C2—C3	1.3908 (19)	C13—C21	1.4278 (17)
C2—C7	1.4057 (18)	C14—O1	1.2347 (14)
C3—C4	1.364 (2)	C14—C15	1.4680 (18)
C3—H3	0.9300	C15—C20	1.4025 (18)
C4—C5	1.391 (2)	C15—C16	1.4079 (19)
C4—H4	0.9300	C16—O2	1.3458 (16)
C5—C6	1.371 (2)	C16—C17	1.386 (2)

C5—H5	0.9300	C17—C18	1.362 (2)
C6—C7	1.3895 (17)	C17—H17	0.9300
C6—H6	0.9300	C18—C19	1.383 (2)
C7—C8	1.4532 (17)	C18—H18	0.9300
C8—C9	1.4431 (18)	C19—C20	1.3690 (19)
C9—N2	1.3469 (15)	C19—H19	0.9300
C9—C13	1.4199 (16)	C20—H20	0.9300
C10—N2	1.3209 (16)	C21—N3	1.1413 (16)
C10—C11	1.3943 (16)	N1—H1A	0.8600
C10—H10	0.9300	O2—H2	0.8200

N1—C1—C8	110.55 (11)	C13—C12—C11	120.06 (11)
N1—C1—H1	124.7	C13—C12—H12	120.0
C8—C1—H1	124.7	C11—C12—H12	120.0
N1—C2—C3	129.31 (13)	C12—C13—C9	120.04 (11)
N1—C2—C7	107.86 (12)	C12—C13—C21	117.84 (10)
C3—C2—C7	122.83 (13)	C9—C13—C21	122.01 (11)
C4—C3—C2	117.03 (15)	O1—C14—C15	120.48 (12)
C4—C3—H3	121.5	O1—C14—C11	117.25 (11)
C2—C3—H3	121.5	C15—C14—C11	122.26 (10)
C3—C4—C5	121.22 (14)	C20—C15—C16	117.50 (12)
C3—C4—H4	119.4	C20—C15—C14	123.11 (12)
C5—C4—H4	119.4	C16—C15—C14	119.38 (11)
C6—C5—C4	121.76 (15)	O2—C16—C17	117.64 (13)
C6—C5—H5	119.1	O2—C16—C15	122.20 (12)
C4—C5—H5	119.1	C17—C16—C15	120.16 (13)
C5—C6—C7	118.83 (14)	C18—C17—C16	120.44 (15)
C5—C6—H6	120.6	C18—C17—H17	119.8
C7—C6—H6	120.6	C16—C17—H17	119.8
C6—C7—C2	118.32 (12)	C17—C18—C19	120.77 (14)
C6—C7—C8	135.38 (12)	C17—C18—H18	119.6
C2—C7—C8	106.30 (11)	C19—C18—H18	119.6
C1—C8—C9	128.49 (11)	C20—C19—C18	119.45 (14)
C1—C8—C7	105.62 (11)	C20—C19—H19	120.3
C9—C8—C7	125.89 (11)	C18—C19—H19	120.3
N2—C9—C13	119.19 (11)	C19—C20—C15	121.61 (14)
N2—C9—C8	116.18 (10)	C19—C20—H20	119.2
C13—C9—C8	124.56 (11)	C15—C20—H20	119.2
N2—C10—C11	125.62 (11)	N3—C21—C13	178.40 (14)
N2—C10—H10	117.2	C1—N1—C2	109.65 (11)
C11—C10—H10	117.2	C1—N1—H1A	125.2
C12—C11—C10	115.75 (11)	C2—N1—H1A	125.2
C12—C11—C14	125.71 (11)	C10—N2—C9	119.27 (10)
C10—C11—C14	118.27 (11)	C16—O2—H2	109.5

N1—C2—C3—C4	178.70 (13)	C8—C9—C13—C12	178.66 (10)
C7—C2—C3—C4	−1.0 (2)	N2—C9—C13—C21	−174.18 (10)
C2—C3—C4—C5	1.0 (2)	C8—C9—C13—C21	2.61 (18)

C3—C4—C5—C6	−0.3 (3)	C12—C11—C14—O1	148.20 (13)
C4—C5—C6—C7	−0.5 (3)	C10—C11—C14—O1	−25.54 (17)
C5—C6—C7—C2	0.5 (2)	C12—C11—C14—C15	−31.12 (18)
C5—C6—C7—C8	179.75 (15)	C10—C11—C14—C15	155.15 (11)
N1—C2—C7—C6	−179.50 (11)	O1—C14—C15—C20	163.36 (13)
C3—C2—C7—C6	0.29 (19)	C11—C14—C15—C20	−17.35 (19)
N1—C2—C7—C8	1.05 (13)	O1—C14—C15—C16	−15.49 (19)
C3—C2—C7—C8	−179.16 (12)	C11—C14—C15—C16	163.80 (12)
N1—C1—C8—C9	−178.21 (11)	C20—C15—C16—O2	−177.12 (13)
N1—C1—C8—C7	1.71 (13)	C14—C15—C16—O2	1.8 (2)
C6—C7—C8—C1	179.03 (14)	C20—C15—C16—C17	3.0 (2)
C2—C7—C8—C1	−1.66 (13)	C14—C15—C16—C17	−178.12 (12)
C6—C7—C8—C9	−1.1 (2)	O2—C16—C17—C18	177.76 (15)
C2—C7—C8—C9	178.26 (10)	C15—C16—C17—C18	−2.3 (2)
C1—C8—C9—N2	−166.77 (11)	C16—C17—C18—C19	0.0 (3)
C7—C8—C9—N2	13.34 (17)	C17—C18—C19—C20	1.7 (3)
C1—C8—C9—C13	16.36 (19)	C18—C19—C20—C15	−0.9 (2)
C7—C8—C9—C13	−163.54 (11)	C16—C15—C20—C19	−1.3 (2)
N2—C10—C11—C12	1.95 (18)	C14—C15—C20—C19	179.78 (13)
N2—C10—C11—C14	176.31 (11)	C8—C1—N1—C2	−1.10 (14)
C10—C11—C12—C13	−2.43 (16)	C3—C2—N1—C1	−179.80 (13)
C14—C11—C12—C13	−176.31 (11)	C7—C2—N1—C1	−0.02 (14)
C11—C12—C13—C9	0.66 (17)	C11—C10—N2—C9	0.53 (18)
C11—C12—C13—C21	176.88 (11)	C13—C9—N2—C10	−2.44 (16)
N2—C9—C13—C12	1.88 (16)	C8—C9—N2—C10	−179.49 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···N3^{i}	0.86	2.15	3.0016 (17)	171
O2—H2···O1	0.82	1.84	2.5653 (14)	146

Symmetry code: (i) −*x*+1, *y*+1/2, −*z*−1/2.