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4-Bromo-3-hydroxy-3-(4-hydroxy-2-oxo-2H-chromen-3-yl)indolin-2-one

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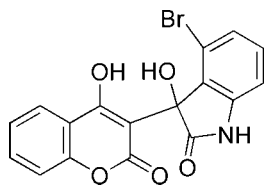
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Key indicators: single-crystal X-ray study; $T = 153$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.024; wR factor = 0.059; data-to-parameter ratio = 12.1.

In the molecule of the title compound, $\text{C}_{17}\text{H}_{10}\text{BrNO}_5$, the indoline system and the attached coumarin ring are each essentially planar with maximum deviations of 0.074 (2) and 0.062 (2) Å, respectively. The dihedral angle between them is 85.09 (3)°. In the crystal, all heteroatoms (except for the coumarin oxo O atoms) are involved in intra- and intermolecular hydrogen bonds. An intramolecular O—H...O hydrogen bond occurs. In the crystal, molecules are linked through O—H...O, N—H...O and C—H...O contacts, forming a complex three-dimensional structure.

Related literature

For general background to indoles and their biological activity, see: Da-Silva *et al.* (2001); Joshi & Chand (1982). Coumarin and its derivatives are important in the perfume, cosmetic and pharmaceutical industries, see: Soine (1964). For the synthesis of indole and coumarin derivatives in water, see: Zhu (2008).



Experimental

Crystal data

$\text{C}_{17}\text{H}_{10}\text{BrNO}_5$
 $M_r = 388.17$
 Monoclinic, $P2_1/c$
 $a = 11.358$ (3) Å
 $b = 13.428$ (3) Å
 $c = 10.360$ (2) Å
 $\beta = 113.307$ (3)°

$V = 1451.1$ (5) Å³
 $Z = 4$
 Mo $K\alpha$ radiation
 $\mu = 2.86$ mm⁻¹
 $T = 153$ K
 $0.78 \times 0.36 \times 0.35$ mm

Data collection

Rigaku Mercury diffractometer
 Absorption correction: multi-scan
 (REQAB; Jacobson, 1998)
 $T_{\min} = 0.173$, $T_{\max} = 0.366$

13755 measured reflections
 2655 independent reflections
 2544 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.023$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.024$
 $wR(F^2) = 0.059$
 $S = 1.08$
 2655 reflections

220 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.34$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.42$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1...O2 ⁱ	0.84	1.98	2.7672 (17)	155
O5—H5...O1	0.84	1.81	2.5486 (19)	145
N1—H1A...O4 ⁱⁱ	0.88	2.16	2.940 (2)	148
C7—H7...O2 ⁱⁱⁱ	0.95	2.49	3.429 (2)	172
C8—H8...O1 ⁱⁱⁱ	0.95	2.61	3.217 (2)	122

Symmetry codes: (i) $x, -y + \frac{1}{2}, z - \frac{1}{2}$; (ii) $-x + 2, -y + 1, -z + 1$; (iii) $-x + 2, y + \frac{1}{2}, -z + \frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku/MS, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MS, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEPII* (Johnson, 1976) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BH2329).

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supplementary materials

Acta Cryst. (2011). E67, o307 [doi:10.1107/S1600536811000213]

4-Bromo-3-hydroxy-3-(4-hydroxy-2-oxo-2H-chromen-3-yl)indolin-2-one

S.-L. Zhu

Comment

The indole nucleus is a well known heterocycle (Da-Silva *et al.*, 2001). Compounds carrying the indole moiety exhibit antibacterial and fungicidal activities (Joshi & Chand, 1982). Coumarin and its derivatives are natural compounds and are also important chemicals in the perfume, cosmetic and pharmaceutical industries (Soine, 1964). As our interest in the synthesis of heterocyclic compounds, guided by the observation that the presence of two or more different heterocyclic moieties in a single molecule often remarkably enhances the biocidal profile, we investigated a simple and green protocol for the synthesis of indole and coumarin derivatives in water (Zhu, 2008). We report herein the crystal structure of the title compound.

In the molecule (Fig. 1), the indole ring (C1...C4/N1/C5...C8) and the attached coumarin ring (C9...C17/O3), are both planar. The dihedral angle between them is 85.09 (3)°. In the crystal structure, intermolecular and intramolecular O—H...O, N—H...O and C—H...O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

The title compound was prepared by the reaction of 4-bromoisatin (4-bromoindole-2,3-dione, 2 mmol) and 4-hydroxy-2H-chromen-2-one (2 mmol) in water (10 ml). The reaction was catalyzed by TEBAC (triethylbenzylammonium chloride, 1 mmol). After stirring at 333 K for 3 h, the reaction mixture was cooled and washed with small amount of ethanol. The crude product was filtered and single crystals of the title compound were obtained from an ethanol solution by slow evaporation at room temperature (yield: 80%; m.p. 469–471 K). Spectroscopic analysis: IR (KBr, ν , cm^{-1}): 3401, 3368, 3251, 3177, 2955, 1710, 1673, 1613, 1520, 1478, 1314, 1231, 1165, 1057, 922, 756, 612, 568. $^1\text{H-NMR}$ (400 MHz, $\text{DMSO-}d_6$): 9.88 (br s, 1H, NH), 7.84 (t, $J = 7.2$ Hz, 1H, ArH), 7.58-6.64 (m, 2H, ArH), 6.75-6.82 (m, 2H, ArH), 6.52- 6.59(m, 2H, ArH), 2.41(s, 1H, OH).

Refinement

H atoms were positioned geometrically, with N—H = 0.88 Å (for NH), O—H = 0.84 Å (for OH) and C—H = 0.95 Å for aromatic H, respectively, and constrained to ride on their parent atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C, N, O})$.

Figures

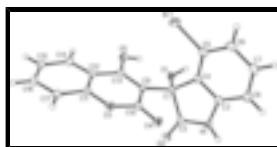


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

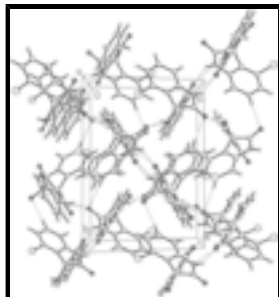


Fig. 2. A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

4-Bromo-3-hydroxy-3-(4-hydroxy-2-oxo-2H-chromen-3-yl)indolin-2-one

Crystal data

$C_{17}H_{10}BrNO_5$

$M_r = 388.17$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 11.358 (3) \text{ \AA}$

$b = 13.428 (3) \text{ \AA}$

$c = 10.360 (2) \text{ \AA}$

$\beta = 113.307 (3)^\circ$

$V = 1451.1 (5) \text{ \AA}^3$

$Z = 4$

$F(000) = 776$

$D_x = 1.777 \text{ Mg m}^{-3}$

Melting point = 469–471 K

Mo $K\alpha$ radiation, $\lambda = 0.71070 \text{ \AA}$

Cell parameters from 5845 reflections

$\theta = 3.0\text{--}25.3^\circ$

$\mu = 2.86 \text{ mm}^{-1}$

$T = 153 \text{ K}$

Block, colourless

$0.78 \times 0.36 \times 0.35 \text{ mm}$

Data collection

Rigaku Mercury
diffractometer

Radiation source: fine-focus sealed tube
graphite

Detector resolution: $7.31 \text{ pixels mm}^{-1}$

ω scans

Absorption correction: multi-scan
(REQAB; Jacobson, 1998)

$T_{\min} = 0.173$, $T_{\max} = 0.366$

13755 measured reflections

2655 independent reflections

2544 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.023$

$\theta_{\max} = 25.4^\circ$, $\theta_{\min} = 3.0^\circ$

$h = -13 \rightarrow 11$

$k = -16 \rightarrow 16$

$l = -12 \rightarrow 12$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.024$

$wR(F^2) = 0.059$

$S = 1.08$

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

$w = 1/[\sigma^2(F_o^2) + (0.0278P)^2 + 1.0659P]$

where $P = (F_o^2 + 2F_c^2)/3$

2655 reflections $(\Delta/\sigma)_{\max} = 0.001$
 220 parameters $\Delta\rho_{\max} = 0.34 \text{ e } \text{\AA}^{-3}$
 0 restraints $\Delta\rho_{\min} = -0.42 \text{ e } \text{\AA}^{-3}$
 0 constraints

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.618858 (19)	0.424530 (16)	-0.05888 (2)	0.02468 (8)
O1	0.81967 (12)	0.24579 (9)	0.19817 (13)	0.0150 (3)
H1	0.8602	0.2544	0.1466	0.023*
O2	0.93364 (12)	0.28564 (10)	0.50987 (13)	0.0165 (3)
O3	0.55747 (12)	0.43528 (9)	0.37776 (13)	0.0147 (3)
O4	0.75296 (12)	0.48622 (9)	0.41805 (13)	0.0170 (3)
O5	0.58573 (13)	0.20063 (10)	0.13673 (14)	0.0195 (3)
H5	0.6572	0.1978	0.1306	0.029*
N1	1.01146 (14)	0.40717 (11)	0.40768 (16)	0.0144 (3)
H1A	1.0875	0.4158	0.4757	0.017*
C1	0.81079 (17)	0.33888 (13)	0.26299 (18)	0.0122 (4)
C2	0.92400 (17)	0.33989 (13)	0.41181 (19)	0.0130 (4)
C3	0.96558 (18)	0.46179 (14)	0.28075 (19)	0.0149 (4)
C4	0.84479 (18)	0.42644 (13)	0.19296 (19)	0.0131 (4)
C5	0.78170 (18)	0.47149 (14)	0.06449 (19)	0.0169 (4)
C6	0.8382 (2)	0.55024 (15)	0.0235 (2)	0.0223 (4)
H6	0.7943	0.5817	-0.0648	0.027*
C7	0.9589 (2)	0.58249 (15)	0.1123 (2)	0.0239 (5)
H7	0.9975	0.6359	0.0832	0.029*
C8	1.02526 (19)	0.53885 (15)	0.2429 (2)	0.0196 (4)
H8	1.1081	0.5613	0.3034	0.023*
C9	0.68273 (17)	0.34335 (13)	0.27623 (18)	0.0124 (4)
C10	0.66978 (17)	0.42446 (13)	0.35962 (19)	0.0124 (4)
C11	0.45996 (17)	0.36647 (14)	0.32443 (18)	0.0135 (4)
C12	0.46973 (17)	0.28643 (14)	0.24491 (18)	0.0139 (4)
C13	0.58467 (17)	0.27702 (14)	0.21777 (18)	0.0136 (4)
C14	0.37095 (18)	0.21509 (15)	0.20037 (19)	0.0176 (4)
H14	0.3758	0.1597	0.1457	0.021*
C15	0.26732 (18)	0.22596 (16)	0.2364 (2)	0.0203 (4)
H15	0.2014	0.1772	0.2084	0.024*
C16	0.25902 (18)	0.30829 (16)	0.3140 (2)	0.0214 (4)
H16	0.1864	0.3156	0.3370	0.026*
C17	0.35425 (18)	0.37954 (15)	0.35806 (19)	0.0178 (4)
H17	0.3476	0.4360	0.4100	0.021*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.02298 (13)	0.02838 (13)	0.01533 (12)	-0.00237 (8)	-0.00025 (9)	0.00135 (8)
O1	0.0179 (7)	0.0140 (7)	0.0178 (7)	-0.0007 (5)	0.0120 (5)	-0.0031 (5)

supplementary materials

O2	0.0181 (7)	0.0185 (7)	0.0146 (6)	0.0034 (5)	0.0084 (5)	0.0029 (5)
O3	0.0115 (6)	0.0166 (7)	0.0166 (7)	-0.0005 (5)	0.0061 (5)	-0.0045 (5)
O4	0.0156 (7)	0.0151 (7)	0.0192 (7)	-0.0024 (5)	0.0058 (5)	-0.0056 (5)
O5	0.0166 (7)	0.0213 (7)	0.0231 (7)	-0.0047 (6)	0.0106 (6)	-0.0118 (6)
N1	0.0099 (7)	0.0185 (8)	0.0131 (8)	-0.0012 (6)	0.0028 (6)	-0.0004 (6)
C1	0.0130 (9)	0.0116 (9)	0.0125 (9)	-0.0004 (7)	0.0057 (7)	-0.0017 (7)
C2	0.0125 (9)	0.0130 (9)	0.0157 (9)	0.0032 (7)	0.0078 (7)	-0.0013 (7)
C3	0.0159 (9)	0.0154 (9)	0.0153 (9)	0.0010 (7)	0.0082 (7)	-0.0021 (8)
C4	0.0153 (9)	0.0122 (9)	0.0143 (9)	-0.0005 (7)	0.0085 (8)	-0.0019 (7)
C5	0.0192 (10)	0.0174 (10)	0.0139 (9)	0.0005 (8)	0.0064 (8)	-0.0024 (8)
C6	0.0326 (12)	0.0192 (10)	0.0158 (10)	0.0000 (9)	0.0101 (9)	0.0038 (8)
C7	0.0338 (12)	0.0179 (10)	0.0256 (11)	-0.0060 (9)	0.0177 (10)	0.0002 (8)
C8	0.0204 (10)	0.0182 (10)	0.0226 (10)	-0.0061 (8)	0.0113 (8)	-0.0035 (8)
C9	0.0121 (9)	0.0136 (9)	0.0112 (9)	0.0009 (7)	0.0045 (7)	-0.0002 (7)
C10	0.0114 (9)	0.0141 (9)	0.0110 (9)	0.0008 (7)	0.0038 (7)	0.0018 (7)
C11	0.0111 (9)	0.0177 (9)	0.0089 (8)	-0.0008 (7)	0.0010 (7)	0.0011 (7)
C12	0.0128 (9)	0.0173 (9)	0.0102 (8)	0.0001 (7)	0.0031 (7)	0.0021 (7)
C13	0.0164 (9)	0.0137 (9)	0.0103 (8)	0.0012 (7)	0.0048 (7)	-0.0003 (7)
C14	0.0176 (9)	0.0185 (10)	0.0155 (9)	-0.0021 (8)	0.0051 (8)	-0.0023 (8)
C15	0.0129 (9)	0.0272 (11)	0.0191 (10)	-0.0068 (8)	0.0045 (8)	-0.0005 (8)
C16	0.0138 (9)	0.0339 (12)	0.0181 (10)	0.0004 (8)	0.0080 (8)	0.0008 (9)
C17	0.0153 (9)	0.0238 (10)	0.0143 (9)	0.0033 (8)	0.0056 (8)	-0.0016 (8)

Geometric parameters (\AA , $^\circ$)

Br1—C5	1.8925 (19)	C6—C7	1.384 (3)
O1—C1	1.441 (2)	C6—H6	0.9500
O1—H1	0.8400	C7—C8	1.392 (3)
O2—C2	1.219 (2)	C7—H7	0.9500
O3—C10	1.369 (2)	C8—H8	0.9500
O3—C11	1.379 (2)	C9—C13	1.366 (3)
O4—C10	1.222 (2)	C9—C10	1.434 (2)
O5—C13	1.329 (2)	C11—C12	1.385 (3)
O5—H5	0.8400	C11—C17	1.387 (3)
N1—C2	1.356 (2)	C12—C14	1.407 (3)
N1—C3	1.413 (2)	C12—C13	1.446 (3)
N1—H1A	0.8800	C14—C15	1.376 (3)
C1—C4	1.510 (2)	C14—H14	0.9500
C1—C9	1.515 (2)	C15—C16	1.392 (3)
C1—C2	1.569 (2)	C15—H15	0.9500
C3—C8	1.376 (3)	C16—C17	1.379 (3)
C3—C4	1.395 (3)	C16—H16	0.9500
C4—C5	1.377 (3)	C17—H17	0.9500
C5—C6	1.388 (3)		
C1—O1—H1	109.5	C3—C8—C7	117.08 (18)
C10—O3—C11	121.22 (14)	C3—C8—H8	121.5
C13—O5—H5	109.5	C7—C8—H8	121.5
C2—N1—C3	111.72 (15)	C13—C9—C10	120.16 (16)
C2—N1—H1A	124.1	C13—C9—C1	125.27 (16)

C3—N1—H1A	124.1	C10—C9—C1	114.56 (15)
O1—C1—C4	111.91 (14)	O4—C10—O3	116.09 (16)
O1—C1—C9	108.86 (14)	O4—C10—C9	124.78 (17)
C4—C1—C9	116.74 (15)	O3—C10—C9	119.13 (15)
O1—C1—C2	106.50 (14)	O3—C11—C12	121.17 (16)
C4—C1—C2	101.50 (14)	O3—C11—C17	116.90 (16)
C9—C1—C2	110.71 (14)	C12—C11—C17	121.91 (17)
O2—C2—N1	126.80 (17)	C11—C12—C14	118.83 (16)
O2—C2—C1	125.59 (16)	C11—C12—C13	118.33 (16)
N1—C2—C1	107.49 (15)	C14—C12—C13	122.75 (17)
C8—C3—C4	122.56 (18)	O5—C13—C9	125.02 (16)
C8—C3—N1	127.83 (17)	O5—C13—C12	115.15 (16)
C4—C3—N1	109.61 (16)	C9—C13—C12	119.82 (16)
C5—C4—C3	118.82 (17)	C15—C14—C12	119.70 (18)
C5—C4—C1	132.24 (17)	C15—C14—H14	120.2
C3—C4—C1	108.91 (16)	C12—C14—H14	120.2
C4—C5—C6	120.25 (18)	C14—C15—C16	120.10 (18)
C4—C5—Br1	120.15 (14)	C14—C15—H15	120.0
C6—C5—Br1	119.59 (15)	C16—C15—H15	120.0
C7—C6—C5	119.43 (19)	C17—C16—C15	121.25 (18)
C7—C6—H6	120.3	C17—C16—H16	119.4
C5—C6—H6	120.3	C15—C16—H16	119.4
C6—C7—C8	121.85 (19)	C16—C17—C11	118.19 (18)
C6—C7—H7	119.1	C16—C17—H17	120.9
C8—C7—H7	119.1	C11—C17—H17	120.9
C3—N1—C2—O2	-176.25 (17)	C2—C1—C9—C13	-125.59 (19)
C3—N1—C2—C1	7.53 (19)	O1—C1—C9—C10	170.24 (14)
O1—C1—C2—O2	-67.8 (2)	C4—C1—C9—C10	-61.9 (2)
C4—C1—C2—O2	175.02 (17)	C2—C1—C9—C10	53.5 (2)
C9—C1—C2—O2	50.4 (2)	C11—O3—C10—O4	-175.77 (15)
O1—C1—C2—N1	108.53 (15)	C11—O3—C10—C9	3.9 (2)
C4—C1—C2—N1	-8.69 (17)	C13—C9—C10—O4	178.59 (17)
C9—C1—C2—N1	-133.29 (15)	C1—C9—C10—O4	-0.5 (3)
C2—N1—C3—C8	176.71 (18)	C13—C9—C10—O3	-1.0 (3)
C2—N1—C3—C4	-3.0 (2)	C1—C9—C10—O3	179.82 (15)
C8—C3—C4—C5	-1.2 (3)	C10—O3—C11—C12	-3.1 (2)
N1—C3—C4—C5	178.55 (16)	C10—O3—C11—C17	174.87 (16)
C8—C3—C4—C1	177.16 (17)	O3—C11—C12—C14	176.13 (16)
N1—C3—C4—C1	-3.1 (2)	C17—C11—C12—C14	-1.7 (3)
O1—C1—C4—C5	71.8 (2)	O3—C11—C12—C13	-0.6 (3)
C9—C1—C4—C5	-54.5 (3)	C17—C11—C12—C13	-178.41 (17)
C2—C1—C4—C5	-174.98 (19)	C10—C9—C13—O5	178.61 (17)
O1—C1—C4—C3	-106.26 (17)	C1—C9—C13—O5	-2.4 (3)
C9—C1—C4—C3	127.40 (17)	C10—C9—C13—C12	-2.5 (3)
C2—C1—C4—C3	6.96 (18)	C1—C9—C13—C12	176.51 (16)
C3—C4—C5—C6	0.4 (3)	C11—C12—C13—O5	-177.70 (16)
C1—C4—C5—C6	-177.55 (18)	C14—C12—C13—O5	5.8 (3)
C3—C4—C5—Br1	179.05 (13)	C11—C12—C13—C9	3.3 (3)
C1—C4—C5—Br1	1.1 (3)	C14—C12—C13—C9	-173.22 (17)

supplementary materials

C4—C5—C6—C7	0.6 (3)	C11—C12—C14—C15	-0.1 (3)
Br1—C5—C6—C7	-178.13 (15)	C13—C12—C14—C15	176.45 (17)
C5—C6—C7—C8	-0.7 (3)	C12—C14—C15—C16	1.4 (3)
C4—C3—C8—C7	1.0 (3)	C14—C15—C16—C17	-1.0 (3)
N1—C3—C8—C7	-178.66 (18)	C15—C16—C17—C11	-0.8 (3)
C6—C7—C8—C3	-0.1 (3)	O3—C11—C17—C16	-175.81 (16)
O1—C1—C9—C13	-8.8 (2)	C12—C11—C17—C16	2.1 (3)
C4—C1—C9—C13	119.0 (2)		

Hydrogen-bond geometry (\AA , $^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
O1—H1 \cdots O2 ⁱ	0.84	1.98	2.7672 (17)	155
O5—H5 \cdots O1	0.84	1.81	2.5486 (19)	145
N1—H1A \cdots O4 ⁱⁱ	0.88	2.16	2.940 (2)	148
C7—H7 \cdots O2 ⁱⁱⁱ	0.95	2.49	3.429 (2)	172
C8—H8 \cdots O1 ⁱⁱⁱ	0.95	2.61	3.217 (2)	122

Symmetry codes: (i) $x, -y+1/2, z-1/2$; (ii) $-x+2, -y+1, -z+1$; (iii) $-x+2, y+1/2, -z+1/2$.

Fig. 1

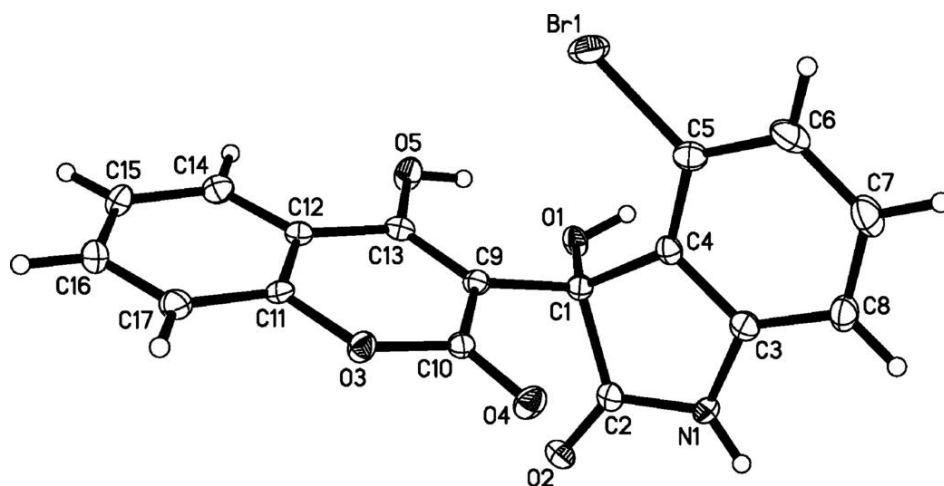


Fig. 2

