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4-Acetamido-2-methoxy-5-[3-(phenylsulfanyl)indole-2-carbonyl]benzoic acid

V. Rajakannan,[a] S. Selvanayagam,[a] M. Yogavel,[a] L. Govindasamy,[a] D. Velmurugan,[a]* S. Shanmuga Sundara Raj,[b] H.-K. Fun[b] and P. C. Srinivasan[c]

[a]Department of Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600025, India, [b]X-ray Crystallographic Unit, Department of Physics, Universiti Sains Malaysia, 11800 USM, Penang, Malaysia, and [c]Department of Organic Chemistry, University of Madras, Guindy Campus, Chennai 600025, India

Correspondence e-mail: d_velu@yahoo.com

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In the title compound, $C_{25}H_{20}N_2O_5S$, the indole ring system is planar. The dihedral angles between the indole moiety and the two substituent aromatic rings are 73.6 (1) and 44.4 (1)°. The structure is influenced by intramolecular O—H···O, N—H···O and C—H···O hydrogen bonds and the crystal structure is stabilized by intermolecular N—H···O hydrogen bonds and C—H···π and C—H···O interactions.

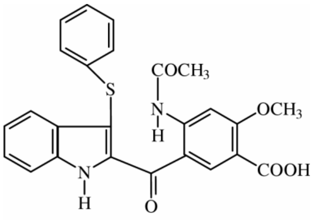
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.045
wR factor = 0.118
Data-to-parameter ratio = 17.2

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

An X-ray study of the title compound, (I), was of interest because indole derivatives exhibit anti-allergic, central nervous system depressant and muscle relaxant properties (Harris & Uhle, 1960; Ho *et al.*, 1986). The indole ring system is present in a number of natural products, many of which are found to possess antidepressant (Grinev *et al.*, 1984), anti-microbial (Gadaginamath & Patil, 1999) and anti-inflammatory (Rodriguez *et al.*, 1985) activities. Indoles have been proved to display high aldose reductose inhibitory activity (Rajeswaran *et al.*, 1999).



(I)

The structure of (I), with the atom-numbering scheme, is shown in Fig. 1. The C—N and C—S bond distances are in good agreement with previously reported values in related structures (Sivaraman *et al.*, 1994*a*,*b*,*c*). The C—O, C═O and C_{phenyl}—C_{phenyl} distances are comparable with the corresponding mean values reported by Allen *et al.* (1987). The geometry of the indole ring system is comparable to our recent findings (Sankaranarayanan *et al.*, 2001; Sankaranarayanan, Yogavel, Velmurugan, Sekar, Babu *et al.*, 2003; Sankaranarayanan, Yogavel, Velmurugan, Sekar, Srinivasan *et al.*, 2003). The sum of the angles around N25 [359.8 (1)°] is indicative of sp^2 hybridization. The exocyclic angles around C20 show considerable asymmetry, O4—C20—C21 [121.8 (2)°] being wider than O4—C20—C19 [116.4 (1)°]. This may be due to the steric repulsion between H21 and H24*C* separated by 2.22 Å. The conformation of the attachment of the two aromatic rings to the indole moiety is described by the torsion angles C10—S1—C3—C2 [110.0 (2)°] and C17—C16—C2—N1 [−160.8 (2)°]. The torsion angles C24—O4—C20—C21 [−10.2 (2)°] and C24—O4—C20—C19 [170.1 (2)°] indicate

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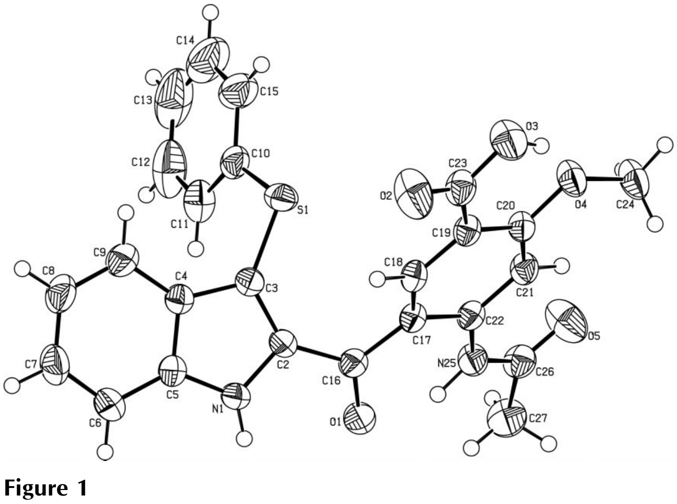

Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

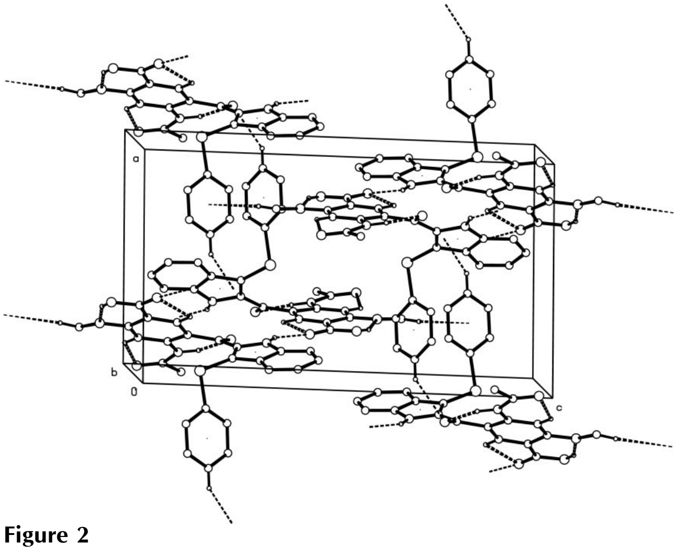

Figure 2
The packing of the molecules, viewed down the b axis. Hydrogen bonds are indicated by dashed lines.

that the methoxy group is nearly coplanar with the attached ring. The dihedral angles between the indole moiety and the two rings A (C10–C15) and B (C17–C22) are 73.6 (1) and 44.4 (1)°, respectively. The dihedral angle between the two rings is 78.2 (1)°.

In the molecular structure, the orientations of the substituents on the ring B are influenced by intramolecular O—H···O, N—H···O and C—H···O hydrogen bonds (Table 2). The crystal structure is stabilized by intermolecular N—H···O hydrogen bonds, C—H···O and C—H···π interactions (Table 2 and Fig. 2). In Table 2, CgA denotes the centroid of ring A.

Experimental

The title compound was prepared by the oxidation of the corresponding 2-benzoylindole derivative by Sarrett reagent, CrO_3–pyridine (Arumugam & Srinivasan, 2003). Single crystals were obtained from methanol by slow evaporation.

Crystal data

$C_{25}H_{20}N_2O_5S$
$M_r = 460.49$
Monoclinic, $P2_1/n$
$a = 10.8499$ (2) Å
$b = 10.5171$ (2) Å
$c = 19.0168$ (3) Å
$\beta = 92.104$ (1)°
$V = 2168.53$ (7) Å^3
$Z = 4$

$D_x = 1.410$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 8224 reflections
$\theta = 2.1$–28.4°
$\mu = 0.19$ mm^{-1}
$T = 293$ (2) K
Block, yellow
0.46 × 0.22 × 0.20 mm

Data collection

Siemens SMART CCD area-detector diffractometer
ω scans
Absorption correction: none
17151 measured reflections
5372 independent reflections

3386 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.074$
$\theta_{\rm max} = 28.4°$
$h = -14 \rightarrow 10$
$k = -14 \rightarrow 14$
$l = -25 \rightarrow 24$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.118$
$S = 0.94$
5372 reflections
312 parameters

H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0564P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} < 0.001$
$\Delta\rho_{\rm max} = 0.24$ e Å^{-3}
$\Delta\rho_{\rm min} = -0.35$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

S1—C3	1.750 (2)	O3—C23	1.334 (2)
S1—C10	1.770 (2)	O4—C20	1.369 (2)
O1—C16	1.235 (2)	O4—C24	1.431 (2)
O2—C23	1.195 (2)	O5—C26	1.204 (2)
C6—C5—C4	122.0 (2)	O4—C20—C19	116.4 (1)
C7—C6—C5	116.8 (2)	C26—N25—C22	128.6 (2)
C6—C7—C8	122.1 (2)	O5—C26—N25	124.1 (2)
C8—C9—C4	118.1 (2)	N25—C26—C27	114.1 (2)
O4—C20—C21	121.8 (2)		
C10—S1—C3—C2	110.0 (2)	C24—O4—C20—C21	−10.2 (2)
N1—C2—C16—C17	−160.8 (2)	C24—O4—C20—C19	170.1 (2)
C2—C16—C17—C18	31.1 (2)		

Table 2
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O3—H3···O4	0.87 (2)	1.78 (3)	2.574 (2)	151 (2)
N25—H25···O1	0.95 (2)	1.89 (2)	2.695 (2)	140 (2)
C18—H18···O2	0.93	2.45	2.770 (2)	100
C21—H21···O5	0.93	2.20	2.826 (2)	124
N1—H1···O2$^{\rm i}$	0.87 (2)	1.99 (2)	2.773 (2)	150 (2)
C13—H13···O1$^{\rm ii}$	0.93	2.59	3.320 (3)	136
C24—H24A···$CgA^{\rm iii}$	0.96	2.89	3.598 (2)	132

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

All C-bound H atoms were positioned geometrically and allowed to ride on their parent atoms and refined isotropically. H atoms attached to N and O were located from a difference Fourier map and refined isotropically. N—H distances are 0.87 (2) and 0.95 (2) Å, and the O—H distance is 0.87 (2) Å.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*3 (Farrugia, 1997) and *PLATON* (Spek, 1990); software used to prepare material for publication: *SHELXL*97 and *PARST* (Nardelli, 1983).

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