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Crystal structure of 5-methoxy-*N'*-(3*Z*)-1-benzyl-5-fluoro-2-oxo-1,2-dihydro-3*H*-indol-3-ylidene]-1*H*-indole-2-carbohydrazide-DMSO (1/1), $C_{27}H_{25}FN_4O_4S$

the atoms including atomic coordinates and displacement parameters.

Table 1: Data collection and handling.

Crystal:	Yellow needle size $0.36 \times 0.06 \times 0.04$ mm
Wavelength:	Mo K_{α} radiation (0.71073 Å)
μ :	1.8 cm^{-1}
Diffractometer, scan mode:	COMS, φ and ω
$2\theta_{\text{max}}$, completeness:	55.2° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	48730, 7452, 0.098
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 4990
$N(\text{param})_{\text{refined}}$:	345
Programs:	Bruker programs [8], SHELXT [9], SHELXL [10]

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Abstract

$C_{27}H_{25}FN_4O_4S$, triclinic, $P\bar{1}$, $a = 10.1996(5)$ Å, $b = 11.4836(6)$ Å, $c = 12.1907(8)$ Å, $\alpha = 100.728(2)^{\circ}$, $\beta = 100.807(2)^{\circ}$, $\gamma = 114.612(2)^{\circ}$, $V = 1218.03(12)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0542$, $wR_{\text{ref}}(F^2) = 0.1319$, $T = 100$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
F1	1.40455(12)	0.84058(11)	0.69213(10)	0.0213(3)
O1	−0.19077(15)	0.03240(14)	0.02158(12)	0.0215(3)
O2	0.65735(14)	0.65059(13)	0.30080(12)	0.0186(3)
O3	0.63232(13)	0.35052(12)	0.55623(11)	0.0144(3)
N1	0.35059(16)	0.49225(15)	0.18665(13)	0.0116(3)
N2	0.64712(17)	0.52240(15)	0.42466(13)	0.0125(3)
N3	0.79770(16)	0.59337(14)	0.47710(13)	0.0118(3)
N4	0.87390(16)	0.42105(15)	0.67376(13)	0.0122(3)
C1	0.20650(19)	0.38943(17)	0.13759(15)	0.0108(3)
C2	0.0871(2)	0.37835(18)	0.05135(16)	0.0138(4)
H2A	0.0975	0.4499	0.0192	0.017*
C3	−0.0463(2)	0.26068(18)	0.01428(16)	0.0152(4)
H3A	−0.1300	0.2514	−0.0431	0.018*
C4	−0.0605(2)	0.15319(18)	0.06053(16)	0.0149(4)
C5	0.0556(2)	0.16447(18)	0.14776(16)	0.0145(4)
H5A	0.0440	0.0924	0.1795	0.017*
C6	0.19169(19)	0.28499(17)	0.18864(15)	0.0119(3)
C7	0.33439(19)	0.33077(18)	0.27221(16)	0.0130(3)
H7A	0.3604	0.2834	0.3211	0.016*
C8	0.42743(19)	0.45736(17)	0.26809(15)	0.0113(3)

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Table 2 (continued)

Atom	x	y	z	U _{iso} [*] /U _{eq}
C9	0.58584(19)	0.55301(17)	0.33080(15)	0.0127(3)
C10	0.85203(19)	0.54961(17)	0.55472(15)	0.0106(3)
C11	1.01003(19)	0.60735(17)	0.62067(15)	0.0112(3)
C12	1.1395(2)	0.71492(17)	0.61911(16)	0.0136(4)
H12A	1.1355	0.7689	0.5696	0.016*
C13	1.2740(2)	0.73923(18)	0.69315(16)	0.0147(4)
C14	1.2841(2)	0.66515(19)	0.76845(16)	0.0167(4)
H14A	1.3795	0.6887	0.8199	0.020*
C15	1.1551(2)	0.55615(18)	0.76914(16)	0.0149(4)
H15A	1.1601	0.5035	0.8198	0.018*
C16	1.01947(19)	0.52761(17)	0.69341(15)	0.0119(3)
C17	0.76857(19)	0.42847(17)	0.59205(15)	0.0113(3)
C18	0.8362(2)	0.32139(18)	0.73717(16)	0.0146(4)
H18A	0.7375	0.3028	0.7504	0.017*
H18B	0.9130	0.3596	0.8147	0.017*
C19	0.8281(2)	0.19028(18)	0.67525(16)	0.0134(4)
C20	0.6885(2)	0.07723(19)	0.62053(17)	0.0177(4)
H20A	0.5985	0.0837	0.6198	0.021*
C21	0.6795(2)	−0.0447(2)	0.56705(18)	0.0220(4)
H21A	0.5837	−0.1213	0.5306	0.026*
C22	0.8096(2)	−0.0549(2)	0.56671(18)	0.0232(4)
H22A	0.8035	−0.1384	0.5302	0.028*
C23	0.9491(2)	0.0571(2)	0.61987(19)	0.0238(4)
H23A	1.0387	0.0503	0.6192	0.029*
C24	0.9590(2)	0.17925(19)	0.67404(17)	0.0189(4)
H24A	1.0551	0.2555	0.7104	0.023*
C25	−0.2891(2)	0.0012(2)	−0.09161(18)	0.0221(4)
H25A	−0.3622	−0.0943	−0.1186	0.033*
H25B	−0.2298	0.0220	−0.1464	0.033*
H25C	−0.3430	0.0547	−0.0876	0.033*
S1	0.53908(5)	0.81144(5)	0.08539(4)	0.01607(12)
O4	0.39759(15)	0.70642(14)	0.09922(13)	0.0208(3)
C26	0.6464(2)	0.7289(2)	0.04849(18)	0.0213(4)
H26A	0.5907	0.6607	−0.0278	0.032*
H26B	0.6639	0.6859	0.1081	0.032*
H26C	0.7436	0.7947	0.0449	0.032*
C27	0.6595(2)	0.9112(2)	0.22935(18)	0.0244(4)
H27A	0.6135	0.9606	0.2672	0.037*
H27B	0.7576	0.9749	0.2253	0.037*
H27C	0.6737	0.8532	0.2748	0.037*
H1N2	0.598(3)	0.455(2)	0.444(2)	0.025(6)*
H1N1	0.388(3)	0.574(3)	0.168(2)	0.035(7)*

Source of material

A catalytic amount of glacial acetic acid was added to a suspension containing equimolar amounts of 5-methoxy-1*H*-indole-2-carbohydrazide and 1-benzyl-5-fluoro-1*H*-indole-2,3-dione in absolute ethanol. The reaction mixture was heated under reflux for three hours, filtered while hot and the separated solid was washed with ethanol. The solid product was collected and re-crystallized from dimethyl sulfoxide to furnish yellow crystals of the title compound.

Experimental details

C-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation, with $U(H)$ set to 1.2 $U_{eq}(C)$. The H atoms of the methyl group were allowed to rotate with a fixed angle around the C—C bond to best fit the experimental electron density (HFIX 137 in the SHELX program suite [10]), with $U(H)$ set to 1.5 $U_{eq}(O)$.

Discussion

Isatin (1*H*-indol-2,3-dione) is an endogenous compound recognized in many organisms and it exhibited a broad spectrum of pharmacological activities [1–4]. Therefore, it has been extensively utilized for the construction of a variety of compounds showing diverse biological activities [5]. On the other hand, indoles are an important class of heterocycles because they constitute the backbone of ubiquitous natural compounds and the indole derivatives have a broad range of biological activities [6, 7]. The title compound contains both isatin and indole moieties. Therefore, it is expected that it will exhibit diverse pharmacological activities.

The asymmetric unit cell of the title compound contains one independent molecule and one dimethyl sulfoxide molecule. The molecules are packed in the crystal structure via three intermolecular non-classical hydrogen bonds, C1—H1A...O1ⁱ, C7—H7A...O4ⁱⁱ and C27—H27A...O2ⁱⁱⁱ. The H...A distances are 2.32, 2.43 and 2.45 Å, respectively and the angles are 157, 180 and 166°. Symmetry codes: (i) $x+1, y, z$; (ii) $-x+1, y+1/2, -z+1$; (iii) $x-1, y, z$.

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