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2-[(*Z*)-(1-Naphthyl)methylene]benzimidazo[2,1-*b*]-thiazol-3(2*H*)-one

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Key indicators

Single-crystal X-ray study
T = 90 K
Mean σ(C–C) = 0.004 Å
R factor = 0.049
wR factor = 0.109
Data-to-parameter ratio = 15.8

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

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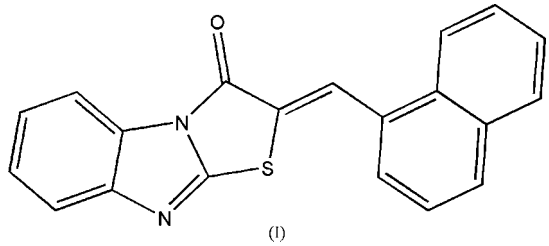
The title compound, $C_{20}H_{12}N_2OS$, was synthesized by mixing 2,4-dichlorobenzaldehyde, ethyl chloroacetate and tetrahydropyrimidine-2-thione in ethanol. The dihedral angle between the naphthalene plane and the heterocyclic ring system is 9.3 (3)°.

Comment

Dihydroimidazoles are reported to exhibit diverse biological and pharmacological properties. Examples of these include vasodepressor, sympathomimetic, antihistaminic, histamine-like and cholinomimetic activity (Gilman & Goodman, 2001; Greenhill & Lue, 1993). Dihydroimidazoles, such as midaglizole, deriglidole and efaroxan, have been found to be potent antihyperglycaemic agents (Bihan *et al.*, 1999). Thus, there has been considerable interest in the chemistry of dihydroimidazole and its derivatives in recent years. In this paper, the structure of the title compound, (I), is reported.



(I)

The molecular structure of (I) is illustrated in Fig. 1. The heterocyclic ring system is essentially planar, with a mean deviation of 0.0067 (3) Å. Selected bond lengths and angles are listed in Table 1. Taking account of the different substitution patterns, the geometry of the heterocyclic ring system compares favourably with that in the related compounds (2*Z*)-2-[(anthracen-9-yl)methylene]-5,6-dihydroimidazo[2,1-*b*]thiazol-3(2*H*)-one (Liang & Li, 2005) and 6-(4-chlorobenzylidene)-2,3-dihydroimidazo[2,1-*b*]thiazol-5(6*H*)-one (Karolak-Wojciechowska & Kieć-Kononowicz, 1991). The naphthalene ring system is planar to within 0.0135 (3) Å. The dihedral angle between the naphthalene plane and the heterocyclic ring system is 9.3 (3)°.

Experimental

A mixture of benz[4,5]imidazo[2,1-*b*]thiazol-3-one (0.02 mol) and naphthaldehyde (0.02 mol) was stirred under reflux in CH_3COONa/CH_3COOH solution (40 ml) for 90 min. After cooling and filtration, the title compound was recrystallized from acetic acid. A quantity of (I) (15 mg) was dissolved in trichloromethane (20 ml) and the solution kept at room temperature for 7 d. Slow solvent evaporation gave

yellow single crystals of (I) suitable for X-ray analysis (m.p. 486–488 K). Spectroscopic analysis: ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.27–7.71 (*m*, 11H, ArH), 7.42 (*s*, 1H, –CH).

Crystal data

$C_{20}H_{12}N_2OS$	D_x = 1.496 Mg m^{-3}
M_r = 328.38	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 894 reflections
a = 6.8627 (16) Å	θ = 3.0–25.4°
b = 7.9031 (19) Å	μ = 0.23 mm^{-1}
c = 27.010 (6) Å	T = 90 (2) K
β = 95.406 (4)°	Plate, yellow
V = 1458.4 (6) Å^3	0.04 × 0.04 × 0.01 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3432 independent reflections
	1989 reflections with $I > 2\sigma(I)$
φ and ω scans	R_{int} = 0.071
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)	θ_{max} = 27.9°
	$h = -8 \rightarrow 8$
T_{min} = 0.980, T_{max} = 0.998	$k = -10 \rightarrow 8$
8139 measured reflections	$l = -28 \rightarrow 35$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.049	$w = 1/[\sigma^2(F_o^2) + (0.0394P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.109	
S = 0.95	$(\Delta/\sigma)_{max} < 0.001$
3432 reflections	$\Delta\rho_{max}$ = 0.34 e Å^{-3}
217 parameters	$\Delta\rho_{min}$ = −0.35 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C1—N2	1.397 (3)	C8—O1	1.212 (3)
C1—C6	1.405 (3)	C8—N2	1.386 (3)
C6—N1	1.418 (3)	C8—C9	1.493 (3)
C7—N1	1.288 (3)	C9—C10	1.334 (3)
C7—N2	1.392 (3)	C9—S1	1.773 (2)
C7—S1	1.740 (3)		
N2—C1—C6	104.1 (2)	N2—C8—C9	108.3 (2)
C1—C6—N1	111.3 (2)	C8—C9—S1	111.72 (17)
N1—C7—N2	115.0 (2)	C7—N1—C6	103.5 (2)
N1—C7—S1	133.0 (2)	C8—N2—C7	117.3 (2)
N2—C7—S1	112.05 (17)	C8—N2—C1	136.6 (2)
O1—C8—N2	124.7 (2)	C7—N2—C1	106.1 (2)
O1—C8—C9	127.0 (2)	C7—S1—C9	90.68 (12)

H atoms were positioned geometrically, with C—H = 0.93–0.98 Å, and refined in a riding model, with U_{iso}(H) = 1.5U_{eq}(carrier).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

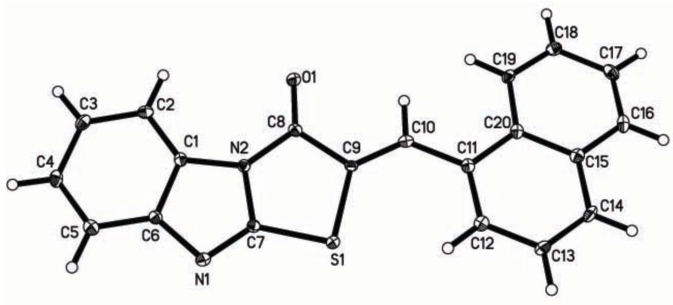


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

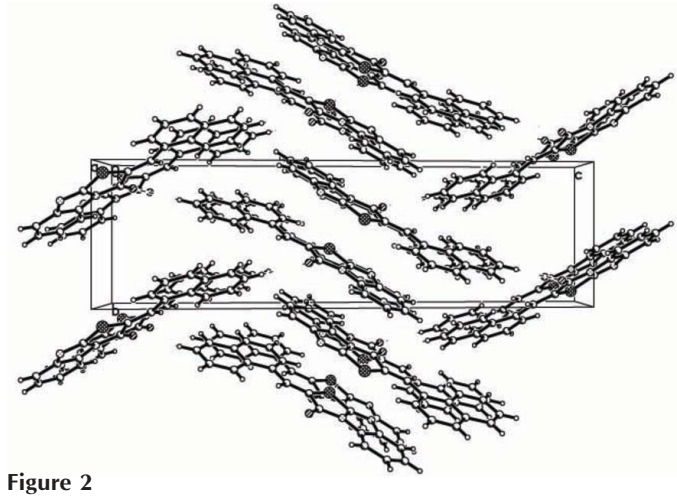


Figure 2
Ihe crystal structure of (I), viewed along the *a* axis.

References

Bihan, G., Rondu, F., Pele, A.-T., Wang, X., Lidy, S., Touboul, E., Lamouri, A., Dive, G., Huet, J., Pfeiffer, B., Renard, P., Guardiola, B.-L., Manechez, D., Penicaud, L., Ktorza, A. & Godfroid, J.-J. (1999). *J. Med. Chem.* **42**, 1587–1592.

Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.

Gilman, A. G. & Goodman, L. S. (2001). *The Pharmacological Basis of Therapeutics*, 10th ed., edited by A.G. Gilman, L. S. Goodman, J. G. Hardman & L. E. Limbird, pp. 215–268. New York: Macmillan.

Greenhill, J. & Lue, P. (1993). Editors. *Progress in Medicinal Chemistry*, pp. 203–326. New York: Elsevier Science.

Karolak-Wojciechowska, J. & Kieć-Kononowicz,K. (1991). *Acta Cryst.* C**47**, 2371–2374.

Liang, Z. P. & Li, J. (2005). *Acta Cryst.* E**60**, o220–o221.

Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.