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3-[(5-Methyl-2-oxo-1,3-benzoxazol-3-yl)methyl]-4-phenyl-1*H*-1,2,4-triazole-5(4*H*)-thione

Yavuz Köysal,[a] Şamil Işık,[a] Umut Salgın[b] and Nesrin Gökhan[b]*

[a]Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey, and [b]Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Hacettepe University, 06100 Sıhhıye Ankara, Turkey
Correspondence e-mail: yavuzk@omu.edu.tr

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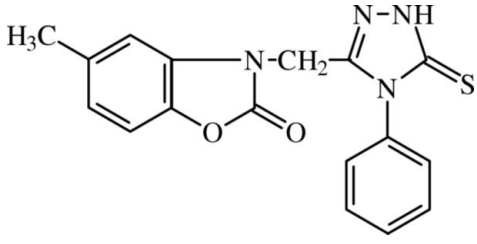
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.109; data-to-parameter ratio = 14.2.

In the title compound, $C_{17}H_{14}N_4O_2S$, the dihedral angle between the triazole ring and the benzoxazoline ring system is 88.20 (4)°, showing that these rings are almost perpendicular to each other. The crystal structure is stabilized by intermolecular N—H···O interactions, linking the molecules into a three-dimensional network.

Related literature

The title compound has a similar appearance to 3-[(5-methyl-2-benzoxazolinone-3-yl)methyl]-4-allyl-1*H*-1,2,4-triazole-5(4*H*)-thione (Köysal *et al.*, 2007). The molecular geometry of the title compound is in agreement with values in our related structures (Köysal *et al.*, 2003, 2007).



Experimental

Crystal data

$C_{17}H_{14}N_4O_2S$
M_r = 338.38
Monoclinic, $P2_1/c$
a = 12.2347 (6) Å
b = 12.8379 (7) Å
c = 11.0797 (6) Å
β = 112.531 (4)°
V = 1607.43 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 293 (2) K
0.54 × 0.39 × 0.24 mm

Data collection

Stoe IPDS II diffractometer
Absorption correction: integration (*X-RED32*; Stoe & Cie, 2002)
T_{min} = 0.484, T_{max} = 0.849
20943 measured reflections
3150 independent reflections
2436 reflections with $I > 2\sigma(I)$
R_{int} = 0.074

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.109
S = 1.03
3150 reflections
222 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

C8—O2	1.206 (2)	N3—N4	1.373 (2)
C10—N4	1.290 (2)		
N1—C9—C10	111.35 (15)		
N1—C9—C10—N2	−163.63 (15)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^{i}	0.86 (2)	1.88 (2)	2.743 (2)	178 (2)

Symmetry code: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PARST* (Nardelli, 1995).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2267).

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supplementary materials

Acta Cryst. (2007). E**63**, o2463 [**doi:10.1107/S1600536807017485**]

3-[(5-Methyl-2-oxo-1,3-benzoxazol-3-yl)methyl]-4-phenyl-1*H*-1,2,4-triazole-5(4*H*)-thione

Y. Köysal, S. Isik, U. Salgin and N. Gökhan

Comment

The structure of the title compound, (I) (Fig. 1), differs from that reported for 3-[(5-methyl-2-benzoxazolinone-3-yl)methyl] -4-allyl-1*H*-1,2,4-triazole-5(4*H*)-thione, (II) (Köysal *et al.*, 2007).

The dihedral angle between the triazole ring and the benzoxazoline ring system is 88.20 (4)°, showing that these ring systems are almost perpendicular to each other. Both compounds (I) and (II) exhibit weak but slightly different intermolecular interactions. In (I), there is an N—H···O interaction, while in (II), the interactions are N—H···S, C—H···S and π–π.

Experimental

The title compound was synthesized using the same procedure as in our previous paper (Köysal *et al.*, 2007).

Refinement

H atoms were located geometrically and refined using a riding model, with C—H = 0.93 Å for aromatic H, 0.97Å for CH_2 and 0.96 Å for methyl H.

Figures

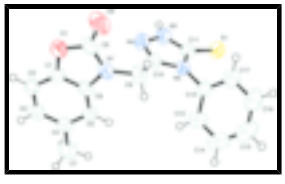

Fig. 1. The structure of compound (I). showing 50% probability displacement ellipsoids and the atom-numbering scheme.

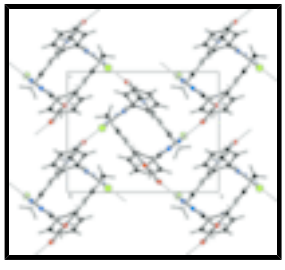

Fig. 2. A view of the intermolecular N—H···O interactions (dashed lines) between the molecules of (I), down the a axis.

3-[(5-Methyl-2-oxo-1,3-benzoxazol-3-yl)methyl]-4-phenyl-1*H*- 1,2,4-triazole-5(4*H*)-thione

Crystal data

$C_{17}H_{14}N_4O_2S$	F_{000} = 704
M_r = 338.38	D_x = 1.398 Mg m^{-3}

Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
Hall symbol: -P 2ybc	Cell parameters from 21935 reflections
$a = 12.2347$ (6) Å	$\theta = 2.4$–28.0°
$b = 12.8379$ (7) Å	$\mu = 0.22$ mm^{-1}
$c = 11.0797$ (6) Å	$T = 293$ (2) K
$\beta = 112.531$ (4)°	Prism, colourless
$V = 1607.43$ (15) Å^3	0.54 × 0.39 × 0.24 mm
$Z = 4$	

Data collection

Stoe IPDS II diffractometer	3150 independent reflections
Radiation source: fine-focus sealed tube	2436 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.074$
Detector resolution: 6.67 pixels mm^{-1}	$\theta_{max} = 26.0^\circ$
$T = 293(2)$ K	$\theta_{min} = 2.4^\circ$
ω scans	$h = -15 \rightarrow 15$
Absorption correction: integration (X-RED32; Stoe & Cie, 2002)	$k = -15 \rightarrow 15$
$T_{min} = 0.484$, $T_{max} = 0.849$	$l = -13 \rightarrow 13$
20943 measured reflections	

Refinement

Refinement on F^2	H atoms treated by a mixture of independent and constrained refinement
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.0405P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.039$	$(\Delta/\sigma)_{max} = 0.002$
$wR(F^2) = 0.109$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
3150 reflections	Extinction correction: none
222 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.92413 (16)	0.44503 (12)	0.32666 (15)	0.0450 (4)
C2	1.02318 (16)	0.39451 (13)	0.40705 (17)	0.0495 (4)
H2	1.0952	0.4001	0.3974	0.059*
C3	1.00960 (17)	0.33420 (13)	0.50425 (17)	0.0512 (4)
H3	1.0744	0.2969	0.5601	0.061*
C4	0.90390 (16)	0.32719 (13)	0.52166 (17)	0.0505 (4)
C5	0.80410 (16)	0.38007 (13)	0.43740 (16)	0.0480 (4)
H5	0.7319	0.3761	0.4470	0.058*
C6	0.81727 (15)	0.43839 (12)	0.33947 (15)	0.0434 (4)
C7	0.8973 (2)	0.26370 (18)	0.6325 (2)	0.0726 (6)
H7A	0.9207	0.1933	0.6255	0.109*
H7B	0.8177	0.2643	0.6289	0.109*
H7C	0.9494	0.2929	0.7141	0.109*
C8	0.79970 (19)	0.54601 (15)	0.17374 (18)	0.0587 (5)
C9	0.61703 (16)	0.52145 (14)	0.21542 (17)	0.0535 (4)
H9A	0.5796	0.4582	0.2284	0.064*
H9B	0.5767	0.5430	0.1252	0.064*
C10	0.60490 (15)	0.60493 (12)	0.30378 (16)	0.0465 (4)
C11	0.52524 (16)	0.71128 (12)	0.40576 (17)	0.0483 (4)
C12	0.39529 (16)	0.56646 (13)	0.27743 (16)	0.0471 (4)
C13	0.3941 (2)	0.46557 (14)	0.31950 (19)	0.0606 (5)
H13	0.4625	0.4353	0.3792	0.073*
C14	0.2889 (2)	0.41019 (17)	0.2710 (2)	0.0742 (6)
H14	0.2868	0.3416	0.2969	0.089*
C15	0.1879 (2)	0.4560 (2)	0.1850 (2)	0.0777 (7)
H15	0.1174	0.4187	0.1534	0.093*
C16	0.1908 (2)	0.5569 (2)	0.1453 (2)	0.0775 (6)
H16	0.1219	0.5879	0.0875	0.093*
C17	0.29451 (18)	0.61215 (16)	0.19043 (19)	0.0612 (5)
H17	0.2966	0.6801	0.1623	0.073*
N1	0.73919 (13)	0.50064 (11)	0.24030 (13)	0.0497 (3)
N2	0.50386 (12)	0.62461 (10)	0.32577 (13)	0.0450 (3)
N3	0.63611 (14)	0.73594 (12)	0.42496 (16)	0.0541 (4)
N4	0.68742 (14)	0.67115 (12)	0.36309 (15)	0.0540 (4)
O1	0.91324 (12)	0.51094 (10)	0.22290 (12)	0.0577 (3)
O2	0.76463 (17)	0.60708 (14)	0.08433 (16)	0.0892 (5)
S1	0.43585 (5)	0.76920 (4)	0.46729 (5)	0.06125 (17)
H3A	0.678 (2)	0.7849 (18)	0.475 (2)	0.064 (6)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0550 (10)	0.0402 (8)	0.0446 (8)	0.0023 (7)	0.0246 (7)	−0.0024 (6)
C2	0.0462 (10)	0.0515 (9)	0.0545 (9)	0.0042 (7)	0.0234 (8)	−0.0051 (7)
C3	0.0482 (10)	0.0496 (9)	0.0508 (9)	0.0072 (7)	0.0136 (7)	0.0001 (7)
C4	0.0541 (11)	0.0461 (9)	0.0506 (9)	0.0016 (7)	0.0191 (8)	0.0031 (7)
C5	0.0468 (10)	0.0442 (8)	0.0557 (9)	−0.0012 (7)	0.0226 (7)	0.0012 (7)
C6	0.0473 (10)	0.0369 (7)	0.0441 (8)	0.0052 (6)	0.0156 (7)	−0.0035 (6)
C7	0.0757 (15)	0.0754 (13)	0.0699 (13)	0.0115 (11)	0.0315 (11)	0.0253 (11)
C8	0.0747 (14)	0.0557 (10)	0.0527 (10)	0.0202 (9)	0.0321 (9)	0.0085 (8)
C9	0.0503 (11)	0.0523 (10)	0.0517 (9)	0.0110 (8)	0.0129 (8)	−0.0056 (8)
C10	0.0450 (10)	0.0432 (8)	0.0491 (9)	0.0077 (7)	0.0156 (7)	0.0016 (7)
C11	0.0529 (11)	0.0389 (8)	0.0539 (9)	0.0010 (7)	0.0213 (8)	−0.0007 (7)
C12	0.0510 (11)	0.0435 (8)	0.0505 (9)	−0.0031 (7)	0.0234 (8)	−0.0043 (7)
C13	0.0740 (14)	0.0496 (10)	0.0611 (11)	−0.0045 (9)	0.0291 (10)	0.0014 (8)
C14	0.1024 (19)	0.0557 (11)	0.0797 (14)	−0.0269 (12)	0.0518 (14)	−0.0117 (10)
C15	0.0731 (16)	0.0910 (17)	0.0760 (14)	−0.0338 (13)	0.0364 (12)	−0.0251 (12)
C16	0.0526 (13)	0.0966 (17)	0.0763 (14)	−0.0113 (11)	0.0167 (10)	−0.0112 (12)
C17	0.0531 (12)	0.0587 (11)	0.0678 (12)	−0.0005 (9)	0.0187 (9)	0.0017 (9)
N1	0.0524 (9)	0.0478 (7)	0.0493 (7)	0.0130 (6)	0.0201 (6)	0.0032 (6)
N2	0.0444 (8)	0.0393 (7)	0.0506 (7)	0.0017 (6)	0.0174 (6)	−0.0012 (5)
N3	0.0494 (9)	0.0474 (8)	0.0661 (9)	−0.0049 (7)	0.0228 (7)	−0.0132 (7)
N4	0.0461 (9)	0.0528 (8)	0.0628 (9)	0.0018 (6)	0.0204 (7)	−0.0095 (7)
O1	0.0681 (9)	0.0596 (7)	0.0556 (7)	0.0148 (6)	0.0352 (6)	0.0106 (6)
O2	0.1090 (14)	0.0961 (11)	0.0760 (10)	0.0471 (10)	0.0503 (9)	0.0423 (9)
S1	0.0609 (3)	0.0541 (3)	0.0784 (3)	−0.0008 (2)	0.0374 (3)	−0.0130 (2)

Geometric parameters (Å, °)

C1—C2	1.362 (2)	C9—H9B	0.9700
C1—C6	1.371 (2)	C10—N4	1.290 (2)
C1—O1	1.3922 (19)	C10—N2	1.372 (2)
C2—C3	1.387 (3)	C11—N3	1.328 (2)
C2—H2	0.9300	C11—N2	1.384 (2)
C3—C4	1.382 (3)	C11—S1	1.6689 (18)
C3—H3	0.9300	C12—C17	1.372 (3)
C4—C5	1.396 (2)	C12—C13	1.379 (2)
C4—C7	1.502 (3)	C12—N2	1.436 (2)
C5—C6	1.378 (2)	C13—C14	1.386 (3)
C5—H5	0.9300	C13—H13	0.9300
C6—N1	1.398 (2)	C14—C15	1.371 (4)
C7—H7A	0.9600	C14—H14	0.9300
C7—H7B	0.9600	C15—C16	1.371 (4)
C7—H7C	0.9600	C15—H15	0.9300
C8—O2	1.206 (2)	C16—C17	1.371 (3)
C8—O1	1.360 (2)	C16—H16	0.9300
C8—N1	1.360 (2)	C17—H17	0.9300

C9—N1	1.437 (2)	N3—N4	1.373 (2)
C9—C10	1.497 (2)	N3—H3A	0.86 (2)
C9—H9A	0.9700		
C2—C1—C6	123.21 (15)	N4—C10—C9	123.39 (17)
C2—C1—O1	127.52 (15)	N2—C10—C9	124.74 (15)
C6—C1—O1	109.27 (14)	N3—C11—N2	103.01 (14)
C1—C2—C3	115.61 (16)	N3—C11—S1	128.11 (14)
C1—C2—H2	122.2	N2—C11—S1	128.85 (14)
C3—C2—H2	122.2	C17—C12—C13	121.08 (18)
C4—C3—C2	122.81 (16)	C17—C12—N2	119.57 (16)
C4—C3—H3	118.6	C13—C12—N2	119.35 (17)
C2—C3—H3	118.6	C12—C13—C14	118.6 (2)
C3—C4—C5	120.03 (16)	C12—C13—H13	120.7
C3—C4—C7	119.74 (17)	C14—C13—H13	120.7
C5—C4—C7	120.23 (17)	C15—C14—C13	120.3 (2)
C6—C5—C4	117.04 (16)	C15—C14—H14	119.8
C6—C5—H5	121.5	C13—C14—H14	119.8
C4—C5—H5	121.5	C14—C15—C16	120.1 (2)
C1—C6—C5	121.29 (15)	C14—C15—H15	120.0
C1—C6—N1	105.95 (14)	C16—C15—H15	120.0
C5—C6—N1	132.75 (16)	C17—C16—C15	120.4 (2)
C4—C7—H7A	109.5	C17—C16—H16	119.8
C4—C7—H7B	109.5	C15—C16—H16	119.8
H7A—C7—H7B	109.5	C16—C17—C12	119.5 (2)
C4—C7—H7C	109.5	C16—C17—H17	120.3
H7A—C7—H7C	109.5	C12—C17—H17	120.3
H7B—C7—H7C	109.5	C8—N1—C6	108.72 (15)
O2—C8—O1	122.11 (19)	C8—N1—C9	123.96 (15)
O2—C8—N1	128.9 (2)	C6—N1—C9	127.18 (15)
O1—C8—N1	109.02 (14)	C10—N2—C11	107.44 (14)
N1—C9—C10	111.35 (15)	C10—N2—C12	127.27 (13)
N1—C9—H9A	109.4	C11—N2—C12	125.28 (14)
C10—C9—H9A	109.4	C11—N3—N4	114.19 (15)
N1—C9—H9B	109.4	C11—N3—H3A	126.6 (15)
C10—C9—H9B	109.4	N4—N3—H3A	119.1 (15)
H9A—C9—H9B	108.0	C10—N4—N3	103.60 (15)
N4—C10—N2	111.76 (14)	C8—O1—C1	106.97 (13)
C6—C1—C2—C3	0.4 (2)	C1—C6—N1—C8	−2.22 (18)
O1—C1—C2—C3	179.27 (15)	C5—C6—N1—C8	176.59 (18)
C1—C2—C3—C4	−1.6 (3)	C1—C6—N1—C9	−177.99 (15)
C2—C3—C4—C5	1.7 (3)	C5—C6—N1—C9	0.8 (3)
C2—C3—C4—C7	−177.52 (18)	C10—C9—N1—C8	−94.1 (2)
C3—C4—C5—C6	−0.4 (2)	C10—C9—N1—C6	81.0 (2)
C7—C4—C5—C6	178.76 (17)	N4—C10—N2—C11	0.23 (19)
C2—C1—C6—C5	0.8 (2)	C9—C10—N2—C11	−176.15 (15)
O1—C1—C6—C5	−178.26 (14)	N4—C10—N2—C12	−178.99 (15)
C2—C1—C6—N1	179.81 (15)	C9—C10—N2—C12	4.6 (3)
O1—C1—C6—N1	0.72 (17)	N3—C11—N2—C10	−0.08 (17)

C4—C5—C6—C1	−0.8 (2)	S1—C11—N2—C10	−178.44 (14)
C4—C5—C6—N1	−179.45 (16)	N3—C11—N2—C12	179.15 (15)
N1—C9—C10—N4	20.4 (2)	S1—C11—N2—C12	0.8 (2)
N1—C9—C10—N2	−163.63 (15)	C17—C12—N2—C10	−114.18 (19)
C17—C12—C13—C14	0.7 (3)	C13—C12—N2—C10	65.9 (2)
N2—C12—C13—C14	−179.39 (17)	C17—C12—N2—C11	66.7 (2)
C12—C13—C14—C15	−1.3 (3)	C13—C12—N2—C11	−113.16 (19)
C13—C14—C15—C16	0.7 (3)	N2—C11—N3—N4	−0.1 (2)
C14—C15—C16—C17	0.5 (4)	S1—C11—N3—N4	178.30 (13)
C15—C16—C17—C12	−1.1 (3)	N2—C10—N4—N3	−0.26 (19)
C13—C12—C17—C16	0.5 (3)	C9—C10—N4—N3	176.17 (15)
N2—C12—C17—C16	−179.42 (18)	C11—N3—N4—C10	0.2 (2)
O2—C8—N1—C6	−177.7 (2)	O2—C8—O1—C1	178.11 (19)
O1—C8—N1—C6	2.9 (2)	N1—C8—O1—C1	−2.43 (19)
O2—C8—N1—C9	−1.7 (3)	C2—C1—O1—C8	−178.01 (17)
O1—C8—N1—C9	178.87 (14)	C6—C1—O1—C8	1.03 (18)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O2^{i}	0.86 (2)	1.88 (2)	2.743 (2)	178 (2)

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2.

Fig. 1

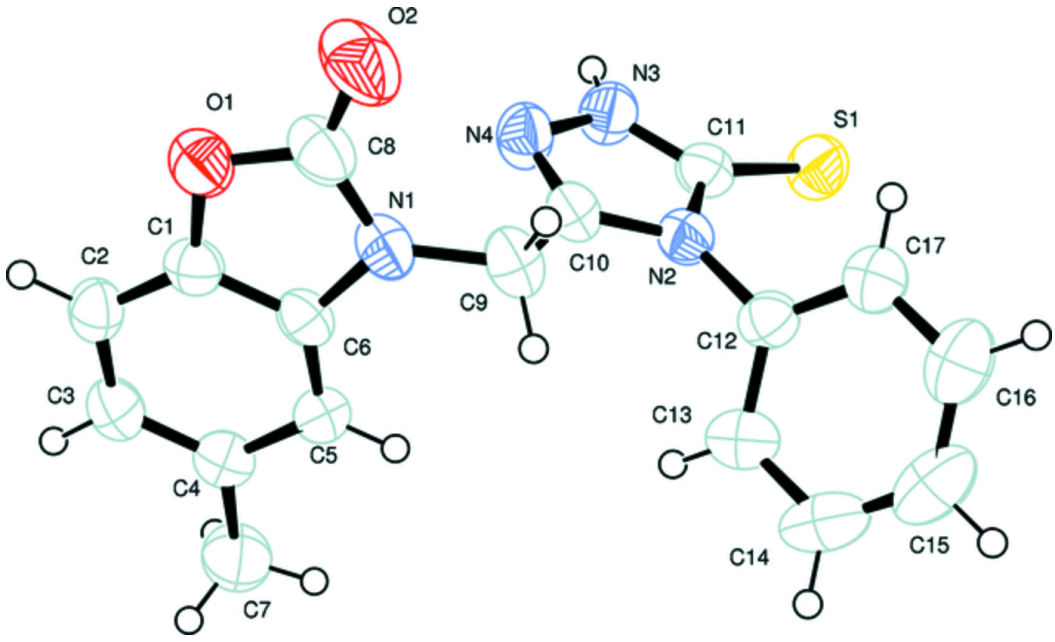
O2
O1
C8
N1
C1
C2
C6
C3
C5
C4
C7
C9
C10
N3
N4
C11
S1
N2
C12
C17
C16
C13
C15
C14

Fig. 2