

Abdullah Aydın,^{a*} Mehmet Akkurt,^b Tijen Önkol^c and Orhan Büyükgüngör^d^aDepartment of Science Education, Faculty of Education, Kastamonu University, 37200 Kastamonu, Turkey, ^bDepartment of Physics, Faculty of Arts and Sciences, Erciyes University, 38039 Kayseri, Turkey, ^cDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Gazi University, 06330 Ankara, Turkey, and ^dDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey

Correspondence e-mail: aaydin@gazi.edu.tr

Key indicators

Single-crystal X-ray study
 $T = 296$ K
Mean $\sigma(C-C) = 0.005$ Å
 R factor = 0.045
 wR factor = 0.123
Data-to-parameter ratio = 14.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

3-[6-(2-Chlorobenzoyl)-2-oxo-2,3-dihydro-1,3-benzothiazol-3-yl]propanenitrile

The title compound, $C_{17}H_{11}ClN_2O_2S$, crystallizes with two crystallographically independent molecules in the asymmetric unit. In the molecular structure, there are intramolecular weak $C-H \cdots O$ hydrogen bonds, which consolidate the molecular conformation.

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Comment

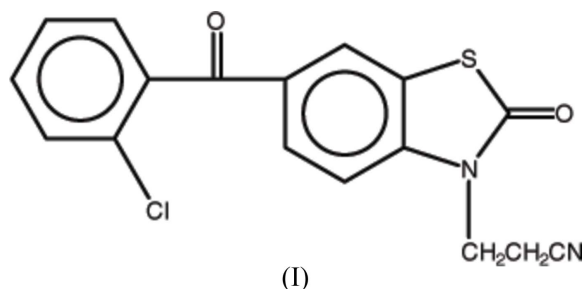
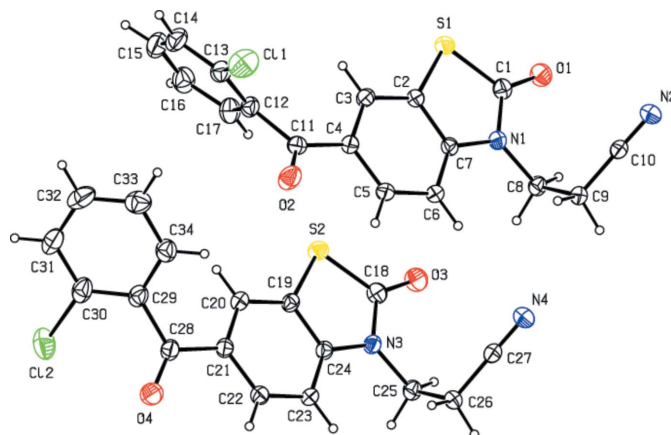
Benzothiazolinone–2-benzoxazolinone derivatives exhibit a variety of pharmacological effects, including analgesic and anti-inflammatory activity (Ferreira *et al.*, 1995; Ünlü *et al.*, 2003). The title compound, (I), is used as an intermediate product in the synthesis of these types of compounds. We report here the crystal structure of (I).The asymmetric unit of (I), which contains two independent molecules, is shown in Fig. 1. The bond lengths and angles have normal values (Allen *et al.*, 1987) and are comparable to those in related structures (Aydın *et al.*, 2003; Işık *et al.*, 2004). The benzothiazole rings in each molecule are essentially planar, with a maximum deviation of 0.019 (1) Å for atom S1

Figure 1

The asymmetric unit of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids.

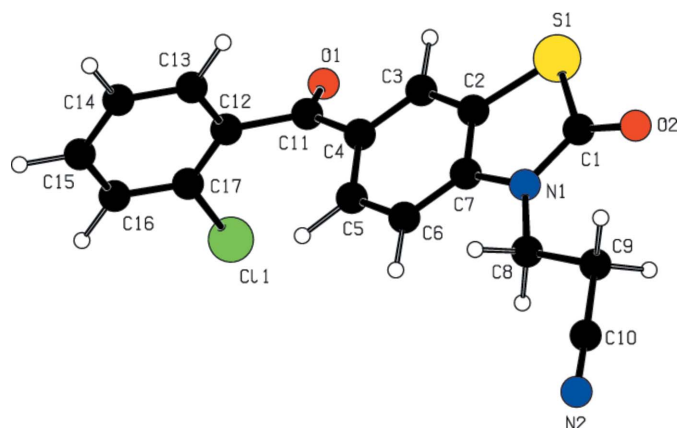


Figure 2
The theoretical structure of the title molecule (I), calculated by the CNDO approximation (Pople & Beveridge, 1970).

in molecule 1 and 0.014 (2) Å for N3 in molecule 2. The planes of these rings in the two molecules make dihedral angles of 69.0 (1) and 63.3 (1)°, respectively, with the C12–C17 and C29–C34 benzene rings. The dihedral angles between the mean planes of the two benzene rings [(C12–C17) and (C29–C34)] and the two benzimidazole rings [(C1–C7/N1/S1) and (C18–C24/N3/S2)], in the asymmetric unit, are 48.7 (2) and 1.45 (8)°, respectively.

A quantum-chemical calculation was performed using the CNDO (Pople & Beveridge, 1970) approximation. A view of the calculated molecule (I) is shown in Fig. 2. The charges at atoms Cl1, S1, N1, N2, O1 and O2 are -0.178 , -0.167 , -0.063 , -0.200 , -0.299 and $-0.400 e^-$, respectively. The calculated dipole moment of (I) is *ca* 5.622 Debye. The HOMO and LUMO energy levels are -10.6709 and $2.4616 eV$, respectively.

The molecular conformation of (I) is stabilized by weak C–H...O intramolecular hydrogen bonds (Table 1).

Experimental

Acylation of 2-benzothiazolinone with 2-chlorobenzoic acid was carried out in polyphosphoric acid as reported in the literature (Çakır *et al.*, 1997). Acrylonitrile (12.0 mmol) was added to a solution of 6-(2-chlorobenzoyl)-2-oxo-1,3-benzothiazol (10.0 mmol) and triethylamine (12.0 mmol) in 50 ml water. After heating (6 h) at 323–333 K while stirring, the mixture was stirred at room temperature for a further 18 h. A solid precipitate formed which was filtered off, washed with water to neutral pH, dried, and crystallized from methanol–water [yield 70%, m.p. 369–370 K (Ünlü *et al.*, 2003)].

Crystal data

$C_{17}H_{11}ClN_2O_2S$
 $M_r = 342.80$
Triclinic, $P\bar{1}$
 $a = 7.089$ (1) Å
 $b = 8.522$ (1) Å
 $c = 26.042$ (2) Å
 $\alpha = 97.724$ (6)°
 $\beta = 91.659$ (6)°
 $\gamma = 93.257$ (6)°

$V = 1555.4$ (3) Å³
 $Z = 4$
 $D_x = 1.464$ Mg m⁻³
Mo $K\alpha$ radiation
 $\mu = 0.39$ mm⁻¹
 $T = 296$ K
Plate, colourless
0.45 × 0.29 × 0.13 mm

Data collection

Stoe IPDS-2 diffractometer
 ω scans
Absorption correction: integration
(*X-RED32*; Stoe & Cie, 2002)
 $T_{min} = 0.844$, $T_{max} = 0.951$

24878 measured reflections
5906 independent reflections
2842 reflections with $I > 2\sigma(I)$
 $R_{int} = 0.085$
 $\theta_{max} = 26.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.045$
 $wR(F^2) = 0.123$
 $S = 0.84$
5906 reflections
416 parameters

H-atom parameters constrained
 $w = 1/[\sigma^2(F_o^2) + (0.0646P)^2]$
where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{max} < 0.001$
 $\Delta\rho_{max} = 0.68 e \text{ \AA}^{-3}$
 $\Delta\rho_{min} = -0.23 e \text{ \AA}^{-3}$

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
C8–H8A...O1	0.97	2.47	2.846 (4)	103
C25–H25A...O3	0.97	2.48	2.852 (4)	103

All H atoms were positioned geometrically [C–H = 0.93 (aromatic) and 0.97 Å (methylene)] and constrained to ride on their parent atoms, with $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED32* (Stoe & Cie, 2002); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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