Ai-Ping Xing, Dai Zeng, Shu-Ling Zhang, Da-Feng Guo and Yi-Xin Chu*

Crystal structure of 3-(benzo[d]thiazol-2-ylamino)isobenzofuran-1(3H)-one, C₁₅H₁₀N₂O₂S

Table 1: Data collection and handling.

Crystal:	Colorless prism
Size:	0.18 × 0.150 × 0.01 mm
Wavelength:	Cu K α radiation (1.54184 Å)
μ :	2.15 mm ⁻¹
Diffractometer, scan mode:	Xcalibur, ω -scans
$\theta_{\max}$, completeness:	70.7°, >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	3447, 1706, 0.028
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1603
$N(\text{param})_{\text{refined}}$:	182
Programs:	CrysAlis ^{PRO} [1], SHELX [2], OLEX2 [3]

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Abstract

C₁₅H₁₀N₂O₂S, monoclinic, *Cc* (no. 9), $a = 10.7988(7)$ Å, $b = 15.7684(10)$ Å, $c = 8.5906(6)$ Å, $\beta = 112.302(8)^\circ$, $V = 1353.38(17)$ Å³, $Z = 4$, $R_{\text{gt}}(F) = 0.0353$, $wR_{\text{ref}}(F^2) = 0.0922$, $T = 293(2)$ K.

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The crystal structure is shown in the figure. Tables 1 and 2 contain details on crystal structure and measurement conditions and a list of the atoms including atomic coordinates and displacement parameters.

Source of material

2-Benzothiazolamine (1.502 g, 10 mmol) and 2-carboxybenzaldehyde (1.491 g, 10 mmol) were mixed in 25 mL ethanol and refluxed for 3 h. When this mixture was cooled to room temperature, a light yellow solid was obtained. Crystallization from methanol gave the title compound as colorless crystals. ¹H NMR (DMSO-d₆, 500 MHz) δ (p.p.m.): 9.36 (d, $J = 9.4$ Hz, 1H), 7.92 (d, $J = 7.6$ Hz, 1H), 7.86 (t, $J = 7.5$ Hz, 1H), 7.81 (dd, $J = 12.6, 8.0$ Hz, 2H), 7.73 (t, $J = 7.4$ Hz, 1H), 7.58 (d, $J = 8.0$ Hz, 1H), 7.39 (d, $J = 9.4$ Hz, 1H), 7.34 (t, $J = 7.7$ Hz, 1H), 7.17 (t, $J = 7.6$ Hz, 1H). ¹³C NMR (DMSO-d₆, 126 MHz) δ (p.p.m.): 169.17, 165.23,

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

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.22070(10)	0.63302(7)	0.34644(12)	0.0536(3)
N1	0.4476(3)	0.5415(2)	0.4453(4)	0.0454(8)
H1A	0.4464	0.5448	0.5446	0.054*
N2	0.3427(3)	0.5755(2)	0.1591(4)	0.0433(8)
O1	0.5088(3)	0.41494(18)	0.3457(3)	0.0512(7)
O2	0.5589(4)	0.2798(2)	0.4199(4)	0.0729(10)
C1	0.7922(5)	0.3605(4)	0.7295(6)	0.0639(13)
H1	0.8027	0.3021	0.7429	0.077*
C2	0.8789(4)	0.4153(4)	0.8440(6)	0.0713(15)
H2	0.9500	0.3936	0.9353	0.086*
C3	0.8619(4)	0.5021(4)	0.8253(6)	0.0665(14)
H3	0.9215	0.5380	0.9046	0.080*
C4	0.7576(4)	0.5365(3)	0.6904(6)	0.0559(11)
H4	0.7462	0.5949	0.6778	0.067*
C5	0.6705(4)	0.4814(3)	0.5748(5)	0.0443(9)
C6	0.6883(4)	0.3954(3)	0.5931(5)	0.0481(9)
C7	0.5831(4)	0.3537(3)	0.4510(5)	0.0501(10)
C8	0.5522(4)	0.4994(3)	0.4179(5)	0.0429(9)
H8	0.5803	0.5329	0.3409	0.051*
C9	0.3476(4)	0.5770(2)	0.3104(4)	0.0406(9)
C10	0.2340(4)	0.6234(2)	0.0541(5)	0.0427(9)
C11	0.1554(4)	0.6598(3)	0.1326(5)	0.0462(9)
C12	0.0439(4)	0.7088(3)	0.0446(6)	0.0587(12)
H12	−0.0084	0.7325	0.0979	0.070*
C13	0.0138(5)	0.7210(3)	−0.1238(6)	0.0636(13)
H13	−0.0600	0.7540	−0.1855	0.076*
C14	0.0910(5)	0.6852(3)	−0.2041(6)	0.0605(12)
H14	0.0682	0.6943	−0.3186	0.073*
C15	0.2013(5)	0.6363(3)	−0.1158(5)	0.0530(11)
H15	0.2529	0.6124	−0.1699	0.064*

*Corresponding author: Yi-Xin Chu, School of Pharmacy, Henan University of Chinese Medicine, Zhengzhou 450046, P.R. China, e-mail: cyxmz2011@126.com

Ai-Ping Xing, Dai Zeng, Shu-Ling Zhang and Da-Feng Guo: School of Pharmacy, Henan University of Chinese Medicine, Zhengzhou 450046, P.R. China

151.84, 145.75, 135.15, 131.33, 131.25, 127.34, 126.47, 125.27, 124.55, 122.88, 121.95, 119.81, 85.53. IR (cm⁻¹, KBr): 3215(br), 3021(w), 2421(m), 1919(w), 1767(s), 1674(s), 1586(m), 1519(s), 1487(m), 1399(m), 1320(s), 1289(s), 1229(m), 1195(w), 1060(s), 1011(w), 780(s), 751(w), 713(s), 687(s), 525(s), 478(w), 431(w).

Experimental details

Hydrogen atoms were placed in their geometrically idealized positions and constrained to ride on their parent atoms.

The Flack-Parsons parameter is 0.020(19) based on only 379 quotients.

Discussion

Antioxidants have received great attention due to their widespread applications in reducing oxidative damage caused by reactive free radical [4]. Some enzymes play an important role in protecting human bodies from being injured by free radicals [5, 6]. It is noteworthy that non-enzymes have been reported to possess antioxidant activities, including phenolic compounds [7], chalcone derivatives, phthalimide derivatives [8–10] and, coordination compounds [11–13]. Although the antioxidant activity of various types of compounds have been well examined, challenges still remain in exploring more efficient and non-toxic antioxidants with highly specified nutritional and therapeutic properties.

The title compound crystallizes in the monoclinic system with a Cc space group with one molecule in the asymmetric unit. As shown in the figure, the molecule structure consists of a phthalide group and a benzothiazole group linked together by nitrogen atom. The phthalide moiety is nearly planar with the largest deviation for atoms C8 and H8. The dihedral angle between the mean planes of the phthalide group and the benzothiazole ring is 68.8°. The C8–N1 distance of 1.404(5) Å is consistent with a C–N single bond, as in 3-(thiazol-2-ylamino)isobenzofuran-1(3H)-one (C–N 1.418(2) Å) [14].

Weak intermolecular N–H···O hydrogen bonds are observed along the *c* direction, forming a chain. Furthermore, C–H···π interaction are found between carbon atom at 3-position of phthalide moiety and phenyl ring from phthalide moiety. These interactions stabilize the solid state of the title compound.

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