Crystal structure of 6-benzyl-3-(2-(2-morpholinoethoxy)phenyl)-7*H*-thiazolo[3, 2-*b*]-1,2,4-triazin-7-one, $C_{24}H_{24}N_4O_3S$

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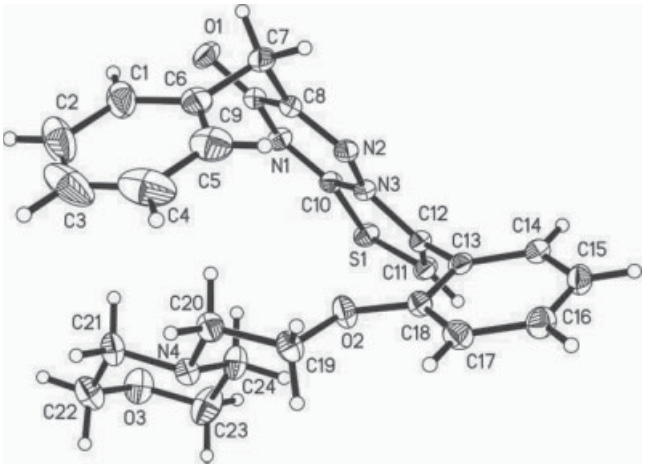

Abstract

$C_{24}H_{24}N_4O_3S$, monoclinic, $P2_1/c$ (no. 14), a = 8.772(2) Å, b = 18.777(4) Å, c = 13.697(3) Å, β = 97.52(3)°, V = 2236.7 Å^3, Z = 4, $R_{gt}(F)$ = 0.0395, $wR_{ref}(F^2)$ = 0.1032, T = 113 K.

Table 1. Data collection and handling.

Crystal:	yellow blocks, size 0.12×0.18×0.20 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.79 cm^{-1}
Diffractometer, scan mode:	Rigaku Saturn, ω
$2\theta_{max}$:	55.02°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	15738, 5131
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 4204
$N(param)_{refined}$:	289
Programs:	SHELX [4]

Source of material

A mixture of 6-benzyl-3-(2-hydroxyphenyl)-7*H*-thiazolo[3,2-*b*]-1,2,4-triazin-7-one (10 mmol), 4-(2-chloroethyl)morpholine hydrochloride (10 mmol), potassium carbonate (50mmol), KI (1 mmol) and acetone (25 ml) was heated under refluxed for 24h. The solvent was evaporated, a residual solid was recrystallized from EtOH.

IR (KBr); $\tilde{\nu}$ 3083, 2851, 2364, 1636, 1478, 1384, 1289, 1264, 1116, 1042, 961, 857, 756, 701 cm^{-1}; **^{1}H-NMR** (300 MHz, DMSO-d_6): δ 7.50 (1H, t), 7.42 (2H, d), 7.22 (5H, m), 7.13 (1H, d), 7.05 (1H, t), 4.00 (2H, t), 3.89 (2H, s), 3.40 (4H, t), 2.36 (2H, t), 2.18 (4H, t); **^{13}C-NMR** (600 MHz, DMSO-d_6): δ 164.1, 159.1, 158.5, 154.0, 135.7, 131.9, 131.6, 130.7, 128.1,127.9, 121.2, 116.9, 113.7, 112.3, 106.7, 67.3, 66.7, 65.4, 57.2, 56.1, 55.3, 35.9.

Discussion

The title compound was synthesized to be used as an acetylcholinesterase inhibitor. This class of compounds display high activities against acetylcholinesterase in vitro [1-3]. The values of the geometric parameters of the title structure are within normal ranges and experimental errors. In the crystal structure, weak intermolecular C–H···O and C–H···N interactions link the molecules, in which they may be effective in the stabilization of the structure. There is also a short intramolecular contact between one of the N atoms of the thiazolo[3,2-*b*]-1,2,4-triazin ring (N3) and the atom O2 bridging the benzene and morpholino moiety.

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(1)	4*e*	–0.4627	0.6768	0.3019	0.046
H(2)	4*e*	–0.5048	0.7717	0.1945	0.068
H(3)	4*e*	–0.4133	0.7689	0.0448	0.077
H(4)	4*e*	–0.2799	0.6703	0.0003	0.068
H(5)	4*e*	–0.2358	0.5748	0.1074	0.046
H(7A)	4*e*	–0.4038	0.5455	0.3183	0.029
H(7B)	4*e*	–0.2934	0.5116	0.2497	0.029
H(11)	4*e*	0.4315	0.5658	0.4853	0.026
H(14)	4*e*	0.3477	0.4244	0.3556	0.026
H(15)	4*e*	0.4183	0.3862	0.2063	0.031
H(16)	4*e*	0.3817	0.4599	0.0707	0.033
H(17)	4*e*	0.2672	0.5706	0.0789	0.031
H(19A)	4*e*	0.0763	0.6493	0.1042	0.030
H(19B)	4*e*	0.2190	0.6985	0.1374	0.030
H(20A)	4*e*	–0.0365	0.7517	0.1371	0.030
H(20B)	4*e*	–0.0452	0.7074	0.2328	0.030
H(21A)	4*e*	–0.0860	0.8155	0.3152	0.034
H(21B)	4*e*	–0.0742	0.8564	0.2165	0.034
H(22A)	4*e*	0.1224	0.9270	0.2940	0.041
H(22B)	4*e*	–0.0217	0.9336	0.3502	0.041
H(23A)	4*e*	0.3199	0.8127	0.4616	0.049
H(23B)	4*e*	0.3306	0.8519	0.3616	0.049
H(24A)	4*e*	0.2687	0.7322	0.3316	0.036
H(24B)	4*e*	0.1217	0.7405	0.3851	0.036

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Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
S(1)	4*e*	0.23256(4)	0.61213(2)	0.56978(2)	0.0191(2)	0.0281(2)	0.0206(2)	–0.0022(1)	0.0017(1)	–0.0031(1)
O(1)	4*e*	–0.3352(1)	0.61949(5)	0.47178(7)	0.0176(5)	0.0345(6)	0.0346(6)	0.0024(4)	0.0081(4)	–0.0023(4)
O(2)	4*e*	0.1774(1)	0.62848(5)	0.24014(7)	0.0392(6)	0.0196(5)	0.0236(5)	0.0077(4)	0.0088(4)	0.0022(4)
O(3)	4*e*	0.1485(1)	0.87860(6)	0.42303(7)	0.0411(7)	0.0367(6)	0.0270(5)	0.0050(5)	0.0006(5)	–0.0096(4)
N(1)	4*e*	–0.0775(1)	0.61829(6)	0.52367(8)	0.0191(6)	0.0253(6)	0.0229(6)	–0.0004(5)	0.0052(5)	–0.0008(4)
N(2)	4*e*	–0.0437(1)	0.54872(6)	0.34324(8)	0.0164(5)	0.0184(5)	0.0232(6)	–0.0024(4)	0.0001(4)	–0.0008(4)
N(3)	4*e*	0.0761(1)	0.56545(6)	0.41361(7)	0.0147(5)	0.0181(5)	0.0205(5)	–0.0013(4)	0.0022(4)	0.0001(4)
N(4)	4*e*	0.1011(1)	0.78875(6)	0.25321(8)	0.0242(6)	0.0203(6)	0.0212(6)	0.0014(5)	0.0021(5)	0.0003(4)
C(1)	4*e*	–0.4253(2)	0.67534(8)	0.2415(1)	0.0321(9)	0.0280(8)	0.050(1)	0.0021(7)	–0.0120(7)	–0.0008(7)
C(2)	4*e*	–0.4506(2)	0.7321(1)	0.1771(2)	0.055(1)	0.0288(9)	0.075(1)	–0.0007(9)	–0.032(1)	0.0034(9)
C(3)	4*e*	–0.3963(3)	0.7304(1)	0.0877(2)	0.071(2)	0.042(1)	0.066(1)	–0.029(1)	–0.040(1)	0.023(1)
C(4)	4*e*	–0.3161(3)	0.6715(1)	0.0611(1)	0.060(1)	0.070(1)	0.0365(9)	–0.033(1)	–0.0150(9)	0.0124(9)
C(5)	4*e*	–0.2898(2)	0.61429(9)	0.1252(1)	0.0365(9)	0.045(1)	0.0315(8)	–0.0125(8)	–0.0060(7)	–0.0004(7)
C(6)	4*e*	–0.3438(2)	0.61593(8)	0.2157(1)	0.0201(7)	0.0269(7)	0.0326(8)	–0.0063(6)	–0.0081(6)	–0.0015(6)
C(7)	4*e*	–0.3133(2)	0.55411(7)	0.2862(1)	0.0172(7)	0.0225(7)	0.0324(7)	–0.0032(6)	0.0004(6)	–0.0030(6)
C(8)	4*e*	–0.1781(2)	0.56852(7)	0.36304(9)	0.0177(6)	0.0162(6)	0.0252(7)	–0.0010(5)	0.0031(5)	0.0022(5)
C(9)	4*e*	–0.2038(2)	0.60437(7)	0.4565(1)	0.0188(7)	0.0184(6)	0.0263(7)	–0.0001(5)	0.0056(5)	0.0019(5)
C(10)	4*e*	0.0562(2)	0.59919(7)	0.49887(9)	0.0183(6)	0.0190(6)	0.0194(6)	–0.0014(5)	0.0037(5)	0.0010(5)
C(11)	4*e*	0.3255(2)	0.57172(7)	0.47965(9)	0.0171(6)	0.0246(7)	0.0244(7)	0.0008(5)	0.0037(5)	0.0005(5)
C(12)	4*e*	0.2295(2)	0.55002(7)	0.40146(9)	0.0153(6)	0.0187(6)	0.0217(6)	0.0002(5)	0.0032(5)	0.0015(5)
C(13)	4*e*	0.2669(2)	0.52071(7)	0.30710(9)	0.0139(6)	0.0209(6)	0.0226(6)	–0.0018(5)	0.0033(5)	–0.0022(5)
C(14)	4*e*	0.3323(2)	0.45380(7)	0.3005(1)	0.0175(6)	0.0221(7)	0.0257(7)	–0.0003(5)	0.0034(5)	0.0004(5)
C(15)	4*e*	0.3746(2)	0.43101(7)	0.2112(1)	0.0248(7)	0.0213(7)	0.0313(7)	0.0029(6)	0.0047(6)	–0.0044(5)
C(16)	4*e*	0.3514(2)	0.47518(7)	0.1299(1)	0.0299(8)	0.0279(7)	0.0256(7)	–0.0002(6)	0.0081(6)	–0.0070(6)
C(17)	4*e*	0.2839(2)	0.54176(7)	0.1345(1)	0.0311(8)	0.0241(7)	0.0230(7)	–0.0014(6)	0.0062(6)	–0.0001(5)
C(18)	4*e*	0.2418(2)	0.56457(7)	0.22373(9)	0.0209(7)	0.0180(6)	0.0253(7)	–0.0003(5)	0.0038(5)	–0.0015(5)
C(19)	4*e*	0.1300(2)	0.67572(7)	0.1591(1)	0.0314(8)	0.0214(7)	0.0221(7)	0.0022(6)	0.0008(6)	0.0022(5)
C(20)	4*e*	0.0248(2)	0.73106(7)	0.1942(1)	0.0247(7)	0.0231(7)	0.0265(7)	0.0001(6)	–0.0019(6)	–0.0008(5)
C(21)	4*e*	–0.0156(2)	0.83934(7)	0.2769(1)	0.0336(8)	0.0248(7)	0.0250(7)	0.0081(6)	0.0013(6)	0.0019(6)
C(22)	4*e*	0.0578(2)	0.90130(8)	0.3343(1)	0.049(1)	0.0246(7)	0.0284(8)	0.0024(7)	0.0060(7)	0.0007(6)
C(23)	4*e*	0.2606(2)	0.8287(1)	0.4008(1)	0.0298(9)	0.051(1)	0.0405(9)	0.0052(8)	–0.0043(7)	–0.0175(8)
C(24)	4*e*	0.1890(2)	0.76511(8)	0.3454(1)	0.0278(8)	0.0307(8)	0.0290(7)	0.0088(6)	–0.0027(6)	–0.0031(6)

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