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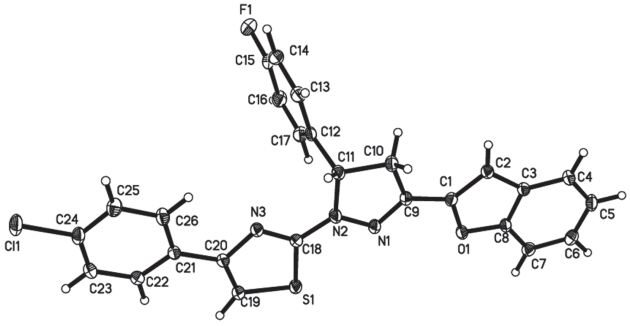
Gamal A. El-Hiti*, Bakr F. Abdel-Wahab, Mohammed Baashen and Hazem A. Ghabbour

Crystal structure of 2-(3-(benzofuran-2-yl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazol-1-yl)-4-(4-chlorophenyl)thiazole, $C_{26}H_{17}ClFN_3OS$



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Abstract

$C_{26}H_{17}ClFN_3OS$, monoclinic, $P2_1/c$ (no. 14), $a = 6.4955(2)$ Å, $b = 14.6143(5)$ Å, $c = 22.6492(8)$ Å, $\beta = 94.568(1)°$, $V = 2143.20(12)$ Å^3, $Z = 4$, $R_{gt}(F) = 0.0461$, $wR_{ref}(F^2) = 0.1069$, $T = 100$ K.

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

***Corresponding author: Gamal A. El-Hiti,** Cornea Research Chair, Department of Optometry, College of Applied Medical Sciences, King Saud University, P. O. Box 10219, Riyadh 11433, Saudi Arabia, e-mail: gelhiti@ksu.edu.sa

Bakr F. Abdel-Wahab: Department of Chemistry, College of Science and Humanities, Shaqra University, Duwadimi, Saudi Arabia; and Applied Organic Chemistry Department, National Research Centre, Dokki, Giza, Egypt

Mohammed Baashen: Department of Chemistry, College of Science and Humanities, Shaqra University, Duwadimi, Saudi Arabia

Hazem A. Ghabbour: Department of Pharmaceutical Chemistry, College of Pharmacy, King Saud University, P. O. Box 2457, Riaydh 11451, Saudi Arabia; and Department of Medicinal Chemistry, Faculty of Pharmacy, University of Mansoura, Mansoura 35516, Egypt

Table 1: Data collection and handling.

Crystal:	Yellow blocks, size 0.547×0.458×0.365 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ	3.1 cm^{-1}
Diffractometer, scan mode:	Bruker Apex-II CCD, φ and ω scans
$2\theta_{max}$, completeness:	65.184°, >99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	30786, 7755, 0.0448
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 5610
$N(param)_{refined}$:	298
Programs:	SHELX [5], Bruker programs [6]

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

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.89879(6)	0.92371(3)	0.14875(2)	0.02728(9)
S1	0.16442(5)	0.94663(3)	0.44387(2)	0.01931(8)
F1	0.73286(14)	0.46836(6)	0.42524(4)	0.0290(2)
O1	0.14074(14)	0.85116(7)	0.66855(4)	0.01721(19)
N1	0.32568(17)	0.86227(8)	0.55935(5)	0.0178(2)
N2	0.46026(18)	0.86166(9)	0.51510(5)	0.0219(3)
N3	0.52699(17)	0.89250(8)	0.41772(5)	0.0175(2)
C1	0.3385(2)	0.81899(9)	0.66240(6)	0.0160(2)
C2	0.4275(2)	0.78481(9)	0.71403(6)	0.0167(2)
H2A	0.5610	0.7583	0.7203	0.020*
C3	0.2799(2)	0.79672(9)	0.75738(6)	0.0159(2)
C4	0.2761(2)	0.77883(10)	0.81808(6)	0.0195(3)
H4A	0.3925	0.7530	0.8401	0.023*
C5	0.0986(2)	0.79975(10)	0.84498(6)	0.0223(3)
H5A	0.0934	0.7878	0.8861	0.027*
C6	−0.0742(2)	0.83815(10)	0.81311(6)	0.0220(3)
H6A	−0.1945	0.8511	0.8328	0.026*
C7	−0.0721(2)	0.85755(10)	0.75317(6)	0.0191(3)
H7A	−0.1880	0.8839	0.7312	0.023*
C8	0.1074(2)	0.83660(9)	0.72706(6)	0.0158(2)
C9	0.4239(2)	0.82796(9)	0.60615(6)	0.0166(2)
C10	0.6445(2)	0.80127(11)	0.59801(6)	0.0211(3)
H10A	0.6722	0.7371	0.6102	0.025*
H10B	0.7434	0.8420	0.6208	0.025*
C11	0.6565(2)	0.81357(10)	0.53069(6)	0.0187(3)
H11A	0.7759	0.8537	0.5228	0.022*
C12	0.67185(19)	0.72325(10)	0.49883(6)	0.0168(3)
C13	0.8669(2)	0.68486(10)	0.49515(6)	0.0206(3)

Table 2: (continued)

	x	*y*	*z*	U_{iso}*/U_{eq}
H13A	0.9862	0.7177	0.5100	0.025*
C14	0.8884(2)	0.59909(11)	0.47003(6)	0.0224(3)
H14A	1.0212	0.5728	0.4675	0.027*
C15	0.7135(2)	0.55314(10)	0.44887(6)	0.0212(3)
C16	0.5174(2)	0.58931(11)	0.45078(6)	0.0233(3)
H16A	0.3990	0.5566	0.4351	0.028*
C17	0.4988(2)	0.67496(11)	0.47633(6)	0.0215(3)
H17A	0.3656	0.7010	0.4785	0.026*
C18	0.4045(2)	0.89612(9)	0.46053(6)	0.0169(3)
C19	0.2370(2)	0.96457(10)	0.37291(6)	0.0190(3)
H19A	0.1528	0.9936	0.3422	0.023*
C20	0.4307(2)	0.93164(9)	0.36684(6)	0.0159(2)
C21	0.5424(2)	0.93008(9)	0.31278(6)	0.0160(2)
C22	0.4496(2)	0.95771(10)	0.25775(6)	0.0210(3)
H22A	0.3100	0.9777	0.2549	0.025*
C23	0.5580(2)	0.95651(10)	0.20727(6)	0.0227(3)
H23A	0.4943	0.9767	0.1703	0.027*
C25	0.8536(2)	0.89421(10)	0.26471(6)	0.0213(3)
H25A	0.9906	0.8710	0.2668	0.026*
C24	0.7601(2)	0.92542(10)	0.21153(6)	0.0200(3)
C26	0.7446(2)	0.89717(10)	0.31515(6)	0.0198(3)
H26A	0.8089	0.8764	0.3519	0.024*

Source of material

Reaction of 3-(benzofuran-2-yl)-5-(4-fluorophenyl)-4,5-dihydro-1*H*-pyrazole-1-carbothioamide and 2-bromo-1-(4-chlorophenyl)ethanone in ethanol under reflux for 3 h provided the crude product. Crystallization from dimethylformamide gave colorless crystals of the title compound (Mp 176–178 °C) [1].

Experimental details

Cell refinement and data reduction were carried out by Bruker SAINT [6].

Discussion

Pyrazolylthiazole derivatives exhibit anti-inflammatory [2], antimicrobial activities [2] and cause antinociception in mice [3]. Also, some derivatives are useful as DF508-cystic fibrosis transmembrane conductance regulators that have improved hydrophilicity compared to bithiazoles [4].

The asymmetric unit of the title structure contains only one independent molecule with a central pyrazol ring (N1/N2/C9—C11) which makes dihedral angles of 1.05 (2)°, 2.85 (2)° and 77.25 (3)° with benzofuran ring (O1/C1—C8), thiazol ring (S1/C18/N3/C19/C20) and fluorophenyl ring (C12—C17), respectively. There is one hydrogen bond: C23—H23A$\cdots$F1^{i} with symmetry code: i = $-x+1$, $y+1/2$, $-z+1/2$.

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