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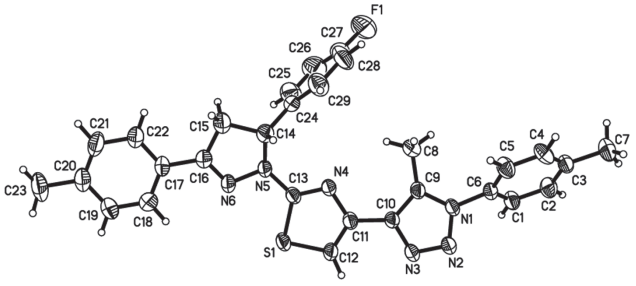
Crystal structure of 2-(5-(4-fluorophenyl)-3-*p*-tolyl-4,5-dihydro-1*H*-pyrazol-1-yl)-4-(5-methyl-1-*p*-tolyl-1*H*-1,2,3-triazol-4-yl)thiazole, $C_{29}H_{25}FN_6S$



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Abstract

$C_{29}H_{25}FN_6S$, triclinic, $P\bar{1}$, $a = 7.5726(8)$ Å, $b = 11.1428(13)$ Å, $c = 16.412(2)$ Å, $\alpha = 91.823(5)°$, $\beta = 102.277(5)°$, $\gamma = 106.692(4)°$, $V = 1289.8(3)$ Å^3, $Z = 2$, $R_{gt}(F) = 0.079$, $wR_{ref}(F^2) = 0.205$, $T = 296$ 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.

Table 1: Data collection and handling.

Crystal:	Yellow block Size 0.39 × 0.28 × 0.13 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	1.6 cm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
$2\theta_{max}$, completeness:	50°, >99%
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	34208, 4526, 0.140
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\,\sigma\,(I_{obs})$, 2673
$N(param)_{refined}$:	337
Programs:	Bruker programs [11], SHELX [12]

Source of material

The title compound was synthesized from reaction of a mixture of 5-(4-fluorophenyl)-3-*p*-tolyl-4,5-dihydro-1*H*-pyrazole-1-carbothioamide and 2-bromo-1-(5-methyl-1-*p*-tolyl-1*H*-1,2,3-triazol-4-yl)ethanone in ethanol under reflux for 2 h. The product obtained was filtered, washed with ethanol and dried to white colorless solid. Crystallization of the crude product using dimethylformamide gave colorless crystals (Mp. 251 °C).

Experimental details

Carbon-bound H atoms were placed in calculated positions and were included in the refinement in the riding model approximation. The H atoms of the methyl groups were allowed to rotate with a fixed angle around the C–C bond to best fit the experimental electron density.

Discussion

Triazole derivatives represent an important class of agrochemicals [1, 2]. Various heterocycles containing triazole ring

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

Atom	x	y	z	U_{iso}*/U_{eq}
S1	0.85746(16)	0.69980(11)	0.84120(8)	0.0448(4)
F1	−0.0226(6)	0.8183(3)	0.4901(2)	0.1089(14)
N1	0.5219(5)	1.1194(3)	0.9068(2)	0.0372(9)
N2	0.6919(5)	1.1447(3)	0.9621(2)	0.0479(10)
N3	0.7573(5)	1.0504(3)	0.9504(2)	0.0493(11)
N4	0.5530(5)	0.7656(3)	0.7976(2)	0.0385(9)
N5	0.5463(5)	0.5815(3)	0.7204(2)	0.0435(10)
N6	0.6402(5)	0.4904(3)	0.7220(2)	0.0414(9)
C1	0.5231(6)	1.3354(4)	0.8980(3)	0.0413(11)
H1A	0.6481	1.3558	0.8930	0.050*
C2	0.4362(7)	1.4282(4)	0.9000(3)	0.0467(12)
H2A	0.5054	1.5115	0.8983	0.056*
C3	0.2497(7)	1.4006(4)	0.9045(3)	0.0424(11)
C4	0.1535(6)	1.2766(5)	0.9091(3)	0.0510(13)
H4A	0.0274	1.2555	0.9126	0.061*
C5	0.2392(6)	1.1829(4)	0.9087(3)	0.0472(12)
H5A	0.1717	1.0997	0.9119	0.057*
C6	0.4245(6)	1.2134(4)	0.9035(3)	0.0345(10)
C7	0.1553(8)	1.5026(5)	0.9075(3)	0.0638(15)
H7A	0.0624	1.4947	0.8561	0.096*
H7B	0.2490	1.5836	0.9147	0.096*
H7C	0.0946	1.4942	0.9537	0.096*
C8	0.3033(6)	0.9556(5)	0.7924(3)	0.0567(14)
H8A	0.3255	0.8992	0.7531	0.085*
H8B	0.2693	1.0226	0.7641	0.085*
H8C	0.2020	0.9106	0.8168	0.085*
C9	0.4787(6)	1.0092(4)	0.8598(3)	0.0348(10)
C10	0.6314(6)	0.9655(4)	0.8881(3)	0.0346(10)
C11	0.6805(6)	0.8554(4)	0.8600(3)	0.0354(10)
C12	0.8482(6)	0.8355(4)	0.8900(3)	0.0414(11)
H12A	0.9457	0.8881	0.9316	0.050*
C13	0.6319(5)	0.6809(4)	0.7818(3)	0.0355(10)
C14	0.3370(6)	0.5240(4)	0.6953(3)	0.0450(12)
H14A	0.2861	0.5138	0.7457	0.054*
C15	0.3238(7)	0.3942(5)	0.6558(4)	0.0628(15)
H15A	0.2323	0.3277	0.6750	0.075*
H15B	0.2888	0.3891	0.5951	0.075*
C16	0.5201(6)	0.3861(4)	0.6859(3)	0.0433(11)
C17	0.5787(7)	0.2728(4)	0.6754(3)	0.0443(11)
C18	0.7573(7)	0.2683(5)	0.7152(3)	0.0574(14)
H18A	0.8416	0.3383	0.7494	0.069*
C19	0.8121(8)	0.1628(5)	0.7050(3)	0.0604(15)
H19A	0.9327	0.1623	0.7325	0.073*
C20	0.6905(8)	0.0567(4)	0.6545(3)	0.0535(13)
C21	0.5130(8)	0.0611(5)	0.6152(4)	0.0647(15)
H21A	0.4292	−0.0087	0.5807	0.078*
C22	0.4561(7)	0.1673(4)	0.6260(3)	0.0579(14)
H22A	0.3345	0.1671	0.5996	0.069*
C23	0.7543(9)	−0.0578(5)	0.6410(4)	0.0796(19)
H23A	0.8397	−0.0666	0.6912	0.119*
H23B	0.8176	−0.0479	0.5957	0.119*
H23C	0.6460	−0.1316	0.6276	0.119*
C24	0.2407(6)	0.6011(4)	0.6389(3)	0.0411(11)
C25	0.2978(7)	0.6449(5)	0.5686(4)	0.0645(15)
H25A	0.4001	0.6256	0.5548	0.077*
C26	0.2090(9)	0.7164(6)	0.5178(4)	0.0743(17)
H26A	0.2496	0.7451	0.4703	0.089*
C27	0.0616(9)	0.7433(5)	0.5390(4)	0.0665(17)
C28	−0.0056(9)	0.6999(6)	0.6048(4)	0.0775(18)
H28A	−0.1114	0.7174	0.6161	0.093*
C29	0.0843(7)	0.6286(5)	0.6558(3)	0.0601(14)
H29A	0.0392	0.5987	0.7020	0.072*

have been synthesized [2–10]. They show a variety of interesting biological activities and can be used as antimicrobial agents [2–10].

The asymmetric unit contains one independent molecule in which the central thiazol ring (C11/C12/S1/C13/N4) makes small dihedral angels 6.11(3)° and 19.13(3)° with triazine (C9/C10/N1/N2/N3) and pyrazol (N5/N6/C14-C16) rings, respectively. The packing structure shows at least one non-classical hydrogen bond between C12—H12A...N3^{i} with a H...N distance of 2.54 Å. Symmetry code: (i) $-x+2$, $-y+2$, $-z+2$.

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