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3-(3,5-Dimethoxyphenyl)-4-(2-methoxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

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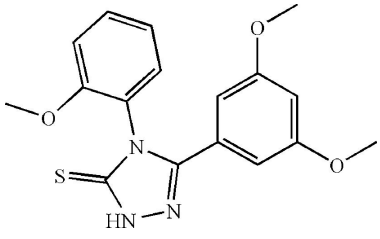
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.035; wR factor = 0.099; data-to-parameter ratio = 16.5.

The title compound, $C_{17}H_{17}N_3O_3S$, is an important biologically active heterocyclic compound containing one five-membered and two six-membered planar rings. The five-membered ring is oriented with respect to the six-membered rings at dihedral angles of 88.84 (2) and 78.69 (3)°. The structure is further stabilized by intermolecular N—H···S stacking interactions.

Related literature

For related literature, see: Demirbas *et al.* (2002); Holla *et al.* (1998); Omar *et al.* (1986); Ozturk *et al.* (2004*a*,*b*); Paulvannan *et al.* (2000); Turan-Zitouni *et al.* (1999); Zhang *et al.* (2004); Kritsanida *et al.* (2002).



Experimental

Crystal data

$C_{17}H_{17}N_3O_3S$
M_r = 343.40
Triclinic, $P\overline{1}$
a = 8.8950 (8) Å
b = 9.3510 (8) Å
c = 10.5510 (9) Å
α = 94.365 (1)°
β = 102.452 (1)°
γ = 108.924 (1)°
V = 800.44 (12) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 100 (2) K
0.35 × 0.30 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.926, T_{max} = 0.946
6943 measured reflections
3963 independent reflections
3136 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.099
S = 1.09
3663 reflections
220 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···S1^{i}	0.88	2.45	3.2624 (12)	154

Symmetry code: (i) $-x+1, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BQ2029).

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supplementary materials

Acta Cryst. (2007). E**63**, o3629 [**doi:10.1107/S1600536807036471**]

3-(3,5-Dimethoxyphenyl)-4-(2-methoxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

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Comment

Substituted triazole derivatives display significant biological activity including antimicrobial (Holla *et al.*, 1998), analgesic (Turan-Zitouni *et al.*, 1999), antitumor (Demirbas *et al.*, 2002), antihypertensive (Paulvannan *et al.*, 2000) and antiviral activities (Kritsanida *et al.*, 2002). The biological activity is closely related to the structure, possibly being due to the presence of the —N—C ═S unit (Omar *et al.*, 1986). We are interested in the synthesis and biological activity of aryloxyacetyl hydrazide derivatives and report here the synthesis and crystal structure of the title compound, (I) (Fig. 1).

The C1═S1 bond length [1.6782 (14) Å] compares with 1.6773 (19) Å in 4-(4-chlorophenyl)-3-(furan-2-yl)-1*H*-1,2,4- triazole-5(4*H*)-thione (Ozturk *et al.*, 2004*a*) and 1.668 (5) Å in 4-amino-3-(1,2,3,4,5-pentahydroxypentyl)-1*H*-1,2,4-triazole- 5(4*H*)-thione (Zhang *et al.*, 2004). In the triazole ring, the N2 ═C1 bond [1.3385 (17) Å] shows double-bond character. In the crystal structure, all bond lengths and angles are comparable with those observed in related structures (Ozturk *et al.*, 2004*a* and 2004*b*). The triazole ring is planar within 0.002 Å and 2-methoxyphenyl ring is almost perpendicular to this ring while 3,5-dimethoxy-phenyl ring is planar to. It forms inversion related dimers *via* N—H···S hydrogen bonds. The structure is further stabilized by intermolecular-stacking interactions down the *b* axis. N2—H2···S1 hydrogen bonds link molecules of title compound into infinite chains extending along the *b* axis of the unit cell (Fig. 2 and Table 1).

Experimental

The synthesis of the title compound was carried out by refluxing a solution of 1-(3,5-dimethoxybenzoyl)-4-(2-methoxyphenyl)thiosemicarbazide (3.47 g, 10 mmol) in 2 *M* NaOH for 5 h. Single crystals suitable for X-ray measurements were obtained by recrystallization from an aqueous ethanol solution at room temperature (yield: 80%; m.p. 470–471 K).

Refinement

The structure was solved by direct methods. H atoms were included in calculated positions with C—H lengths of 0.95(CH), 0.99(CH_2) & 0.98(CH_3)Å; U_{iso}(H) values were fixed at 1.2U_{eq}(C) except for CH_3 where it was 1.5U_{eq}(C).

Figures

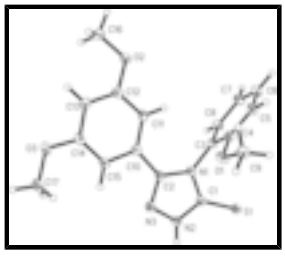


Fig. 1. The molecular structure of (I) with 50% probability displacement ellipsoids (arbitrary spheres for H atoms).

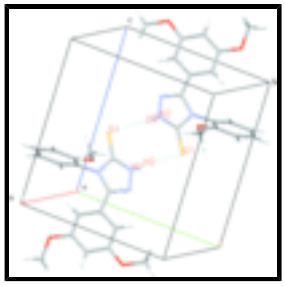


Fig. 2. Crystal packing of (I), showing the formation of hydrogen bonds with the symmetry position $-x + 1, -y + 1, -z + 1$.

Fig. 3. The formation of the title compound.

3-(3,5-Dimethoxyphenyl)-4-(2-methoxyphenyl)-1*H*-1,2,4-triazole-5(4*H*)-thione

Crystal data

$C_{17}H_{17}N_3O_3S$	$Z = 2$
$M_r = 343.40$	$F_{000} = 360$
	$D_x = 1.425$ Mg m^{-3}
Triclinic, $P\overline{1}$	$D_m = 1.411$ Mg m^{-3}
	D_m measured by not measured
Hall symbol: -P 1	Melting point: 470(1) K
$a = 8.8950$ (8) Å	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$b = 9.3510$ (8) Å	Cell parameters from 3874 reflections
$c = 10.5510$ (9) Å	$\theta = 2.3$–28.3°
$\alpha = 94.3650$ (10)°	$\mu = 0.22$ mm^{-1}
$\beta = 102.4520$ (10)°	$T = 100$ (2) K
$\gamma = 108.9240$ (10)°	Block, white
$V = 800.44$ (12) Å^3	0.35 × 0.30 × 0.25 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3963 independent reflections
Radiation source: fine-focus sealed tube	3136 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.031$
$T = 100$(2) K	$\theta_{max} = 28.3^\circ$
φ and ω scans	$\theta_{min} = 2.0^\circ$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -11 \rightarrow 11$
$T_{min} = 0.926$, $T_{max} = 0.946$	$k = -12 \rightarrow 12$
6943 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.035$	H-atom parameters constrained
$wR(F^2) = 0.099$	$w = 1/[\sigma^2(F_o^2) + (0.0582P)^2 + 0.033P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
3625 reflections	$\Delta\rho_{max} = 0.38$ e Å^{-3}
220 parameters	$\Delta\rho_{min} = -0.29$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2$sigma(F^2) is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.55056 (15)	0.34243 (15)	0.35976 (13)	0.0149 (3)
C2	0.65598 (15)	0.41748 (15)	0.19148 (13)	0.0147 (3)
C3	0.67625 (16)	0.17140 (15)	0.27023 (13)	0.0145 (3)
C4	0.84064 (16)	0.19625 (15)	0.33053 (13)	0.0159 (3)
C5	0.89278 (17)	0.07165 (16)	0.33995 (14)	0.0196 (3)
H5	1.0041	0.0864	0.3804	0.024*
C6	0.77988 (17)	−0.07507 (16)	0.28931 (14)	0.0213 (3)
H6	0.8153	−0.1604	0.2961	0.026*
C7	0.61750 (17)	−0.09936 (15)	0.22939 (14)	0.0202 (3)
H7	0.5424	−0.2001	0.1946	0.024*
C8	0.56524 (16)	0.02510 (15)	0.22058 (13)	0.0178 (3)
H8	0.4536	0.0098	0.1806	0.021*
C9	1.10474 (16)	0.37350 (17)	0.44617 (14)	0.0206 (3)
H9A	1.1060	0.3194	0.5222	0.031*
H9B	1.1614	0.4837	0.4763	0.031*
H9C	1.1608	0.3367	0.3876	0.031*
C10	0.72473 (15)	0.42325 (15)	0.07657 (13)	0.0154 (3)
C11	0.75431 (16)	0.30133 (15)	0.01694 (13)	0.0161 (3)
H11	0.7375	0.2092	0.0533	0.019*
C12	0.80932 (16)	0.31619 (15)	−0.09758 (13)	0.0161 (3)
C13	0.83678 (16)	0.45016 (15)	−0.15064 (13)	0.0175 (3)
H13	0.8743	0.4590	−0.2284	0.021*

C14	0.80850 (16)	0.57224 (15)	−0.08796 (13)	0.0175 (3)
C15	0.75216 (16)	0.56080 (15)	0.02409 (13)	0.0167 (3)
H15	0.7322	0.6444	0.0653	0.020*
C16	0.85664 (19)	0.18902 (18)	−0.28188 (14)	0.0243 (3)
H16A	0.7674	0.2106	−0.3401	0.037*
H16B	0.8574	0.0885	−0.3149	0.037*
H16C	0.9620	0.2678	−0.2794	0.037*
C17	0.81545 (19)	0.82927 (16)	−0.08535 (15)	0.0247 (3)
H17A	0.7010	0.8006	−0.0800	0.037*
H17B	0.8398	0.9128	−0.1371	0.037*
H17C	0.8888	0.8630	0.0034	0.037*
N1	0.62267 (13)	0.30080 (12)	0.26679 (10)	0.0138 (2)
N2	0.54324 (13)	0.47840 (13)	0.33425 (11)	0.0164 (2)
H2	0.5009	0.5316	0.3790	0.020*
N3	0.60780 (14)	0.52693 (13)	0.23210 (11)	0.0168 (2)
O1	0.93818 (11)	0.34536 (11)	0.37661 (10)	0.0195 (2)
O2	0.83196 (12)	0.18925 (11)	−0.15200 (9)	0.0186 (2)
O3	0.83978 (13)	0.70006 (11)	−0.14709 (10)	0.0231 (2)
S1	0.48847 (4)	0.24514 (4)	0.47744 (3)	0.01896 (11)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0121 (6)	0.0142 (6)	0.0167 (6)	0.0049 (5)	0.0009 (5)	−0.0004 (5)
C2	0.0132 (6)	0.0118 (6)	0.0171 (6)	0.0037 (5)	0.0011 (5)	0.0025 (5)
C3	0.0165 (6)	0.0135 (6)	0.0159 (6)	0.0076 (5)	0.0046 (5)	0.0037 (5)
C4	0.0164 (6)	0.0144 (6)	0.0158 (6)	0.0044 (5)	0.0036 (5)	0.0015 (5)
C5	0.0175 (6)	0.0193 (7)	0.0222 (7)	0.0085 (5)	0.0020 (5)	0.0031 (6)
C6	0.0245 (7)	0.0163 (7)	0.0265 (7)	0.0112 (6)	0.0061 (6)	0.0054 (6)
C7	0.0211 (7)	0.0117 (6)	0.0261 (7)	0.0040 (5)	0.0054 (6)	0.0029 (5)
C8	0.0158 (6)	0.0157 (7)	0.0213 (7)	0.0049 (5)	0.0044 (5)	0.0031 (5)
C9	0.0154 (6)	0.0217 (7)	0.0209 (7)	0.0053 (5)	−0.0005 (5)	0.0000 (6)
C10	0.0119 (6)	0.0153 (6)	0.0166 (6)	0.0031 (5)	0.0018 (5)	0.0020 (5)
C11	0.0145 (6)	0.0135 (6)	0.0187 (7)	0.0036 (5)	0.0030 (5)	0.0040 (5)
C12	0.0129 (6)	0.0153 (6)	0.0188 (7)	0.0049 (5)	0.0016 (5)	0.0011 (5)
C13	0.0164 (6)	0.0186 (7)	0.0164 (6)	0.0046 (5)	0.0040 (5)	0.0047 (5)
C14	0.0162 (6)	0.0147 (6)	0.0198 (7)	0.0044 (5)	0.0013 (5)	0.0058 (5)
C15	0.0165 (6)	0.0127 (6)	0.0200 (7)	0.0056 (5)	0.0023 (5)	0.0017 (5)
C16	0.0311 (8)	0.0261 (8)	0.0211 (7)	0.0145 (6)	0.0104 (6)	0.0043 (6)
C17	0.0302 (8)	0.0138 (7)	0.0296 (8)	0.0075 (6)	0.0056 (6)	0.0066 (6)
N1	0.0135 (5)	0.0118 (5)	0.0159 (5)	0.0046 (4)	0.0030 (4)	0.0024 (4)
N2	0.0185 (6)	0.0149 (5)	0.0184 (6)	0.0079 (4)	0.0069 (5)	0.0029 (4)
N3	0.0181 (6)	0.0149 (6)	0.0179 (6)	0.0059 (4)	0.0052 (5)	0.0034 (4)
O1	0.0142 (5)	0.0144 (5)	0.0253 (5)	0.0043 (4)	−0.0014 (4)	−0.0017 (4)
O2	0.0230 (5)	0.0164 (5)	0.0198 (5)	0.0089 (4)	0.0088 (4)	0.0038 (4)
O3	0.0321 (6)	0.0154 (5)	0.0249 (5)	0.0092 (4)	0.0101 (4)	0.0092 (4)
S1	0.0240 (2)	0.01631 (18)	0.02032 (19)	0.00884 (14)	0.00978 (14)	0.00527 (13)

Geometric parameters (Å, °)

C1—N2	1.3385 (17)	C10—C11	1.3862 (19)
C1—N1	1.3785 (16)	C10—C15	1.4084 (18)
C1—S1	1.6782 (14)	C11—C12	1.3982 (19)
C2—N3	1.3083 (17)	C11—H11	0.9500
C2—N1	1.3905 (16)	C12—O2	1.3712 (16)
C2—C10	1.4680 (18)	C12—C13	1.3820 (19)
C3—C8	1.3830 (18)	C13—C14	1.3953 (19)
C3—C4	1.3974 (18)	C13—H13	0.9500
C3—N1	1.4374 (16)	C14—O3	1.3667 (16)
C4—O1	1.3651 (15)	C14—C15	1.3786 (19)
C4—C5	1.3896 (19)	C15—H15	0.9500
C5—C6	1.3928 (19)	C16—O2	1.4337 (16)
C5—H5	0.9500	C16—H16A	0.9800
C6—C7	1.3817 (19)	C16—H16B	0.9800
C6—H6	0.9500	C16—H16C	0.9800
C7—C8	1.3885 (18)	C17—O3	1.4289 (17)
C7—H7	0.9500	C17—H17A	0.9800
C8—H8	0.9500	C17—H17B	0.9800
C9—O1	1.4324 (15)	C17—H17C	0.9800
C9—H9A	0.9800	N2—N3	1.3674 (15)
C9—H9B	0.9800	N2—H2	0.8800
C9—H9C	0.9800		
N2—C1—N1	103.64 (11)	C12—C11—H11	120.6
N2—C1—S1	128.55 (10)	O2—C12—C13	123.48 (12)
N1—C1—S1	127.81 (10)	O2—C12—C11	115.21 (12)
N3—C2—N1	110.19 (11)	C13—C12—C11	121.30 (13)
N3—C2—C10	121.30 (12)	C12—C13—C14	118.86 (13)
N1—C2—C10	128.40 (11)	C12—C13—H13	120.6
C8—C3—C4	121.02 (12)	C14—C13—H13	120.6
C8—C3—N1	120.42 (11)	O3—C14—C15	123.94 (12)
C4—C3—N1	118.48 (11)	O3—C14—C13	114.70 (12)
O1—C4—C5	125.09 (12)	C15—C14—C13	121.35 (12)
O1—C4—C3	115.70 (11)	C14—C15—C10	118.93 (12)
C5—C4—C3	119.22 (12)	C14—C15—H15	120.5
C4—C5—C6	119.21 (12)	C10—C15—H15	120.5
C4—C5—H5	120.4	O2—C16—H16A	109.5
C6—C5—H5	120.4	O2—C16—H16B	109.5
C7—C6—C5	121.47 (12)	H16A—C16—H16B	109.5
C7—C6—H6	119.3	O2—C16—H16C	109.5
C5—C6—H6	119.3	H16A—C16—H16C	109.5
C6—C7—C8	119.30 (13)	H16B—C16—H16C	109.5
C6—C7—H7	120.3	O3—C17—H17A	109.5
C8—C7—H7	120.3	O3—C17—H17B	109.5
C3—C8—C7	119.77 (12)	H17A—C17—H17B	109.5
C3—C8—H8	120.1	O3—C17—H17C	109.5
C7—C8—H8	120.1	H17A—C17—H17C	109.5

O1—C9—H9A	109.5	H17B—C17—H17C	109.5
O1—C9—H9B	109.5	C1—N1—C2	107.79 (11)
H9A—C9—H9B	109.5	C1—N1—C3	122.33 (11)
O1—C9—H9C	109.5	C2—N1—C3	128.97 (11)
H9A—C9—H9C	109.5	C1—N2—N3	113.65 (11)
H9B—C9—H9C	109.5	C1—N2—H2	123.2
C11—C10—C15	120.65 (13)	N3—N2—H2	123.2
C11—C10—C2	123.83 (12)	C2—N3—N2	104.73 (11)
C15—C10—C2	115.44 (12)	C4—O1—C9	116.91 (10)
C10—C11—C12	118.89 (12)	C12—O2—C16	116.63 (11)
C10—C11—H11	120.6	C14—O3—C17	116.86 (11)
C8—C3—C4—O1	−179.51 (12)	C11—C10—C15—C14	0.21 (19)
N1—C3—C4—O1	−2.65 (17)	C2—C10—C15—C14	−176.68 (11)
C8—C3—C4—C5	0.3 (2)	N2—C1—N1—C2	0.68 (13)
N1—C3—C4—C5	177.14 (12)	S1—C1—N1—C2	−178.90 (9)
O1—C4—C5—C6	179.63 (13)	N2—C1—N1—C3	170.67 (11)
C3—C4—C5—C6	−0.1 (2)	S1—C1—N1—C3	−8.90 (18)
C4—C5—C6—C7	0.3 (2)	N3—C2—N1—C1	−0.41 (14)
C5—C6—C7—C8	−0.6 (2)	C10—C2—N1—C1	−176.69 (12)
C4—C3—C8—C7	−0.6 (2)	N3—C2—N1—C3	−169.53 (12)
N1—C3—C8—C7	−177.40 (12)	C10—C2—N1—C3	14.2 (2)
C6—C7—C8—C3	0.8 (2)	C8—C3—N1—C1	81.84 (16)
N3—C2—C10—C11	−169.74 (12)	C4—C3—N1—C1	−95.05 (15)
N1—C2—C10—C11	6.2 (2)	C8—C3—N1—C2	−110.45 (15)
N3—C2—C10—C15	7.04 (18)	C4—C3—N1—C2	72.67 (17)
N1—C2—C10—C15	−177.05 (12)	N1—C1—N2—N3	−0.75 (14)
C15—C10—C11—C12	−1.05 (19)	S1—C1—N2—N3	178.82 (9)
C2—C10—C11—C12	175.56 (11)	N1—C2—N3—N2	−0.04 (14)
C10—C11—C12—O2	−178.55 (11)	C10—C2—N3—N2	176.55 (11)
C10—C11—C12—C13	0.99 (19)	C1—N2—N3—C2	0.51 (14)
O2—C12—C13—C14	179.44 (12)	C5—C4—O1—C9	−3.58 (19)
C11—C12—C13—C14	−0.07 (19)	C3—C4—O1—C9	176.19 (11)
C12—C13—C14—O3	179.68 (11)	C13—C12—O2—C16	−11.41 (18)
C12—C13—C14—C15	−0.8 (2)	C11—C12—O2—C16	168.12 (11)
O3—C14—C15—C10	−179.80 (12)	C15—C14—O3—C17	1.57 (19)
C13—C14—C15—C10	0.75 (19)	C13—C14—O3—C17	−178.94 (12)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···S1^{i}	0.88	2.45	3.2624 (12)	154

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1.

Fig. 1

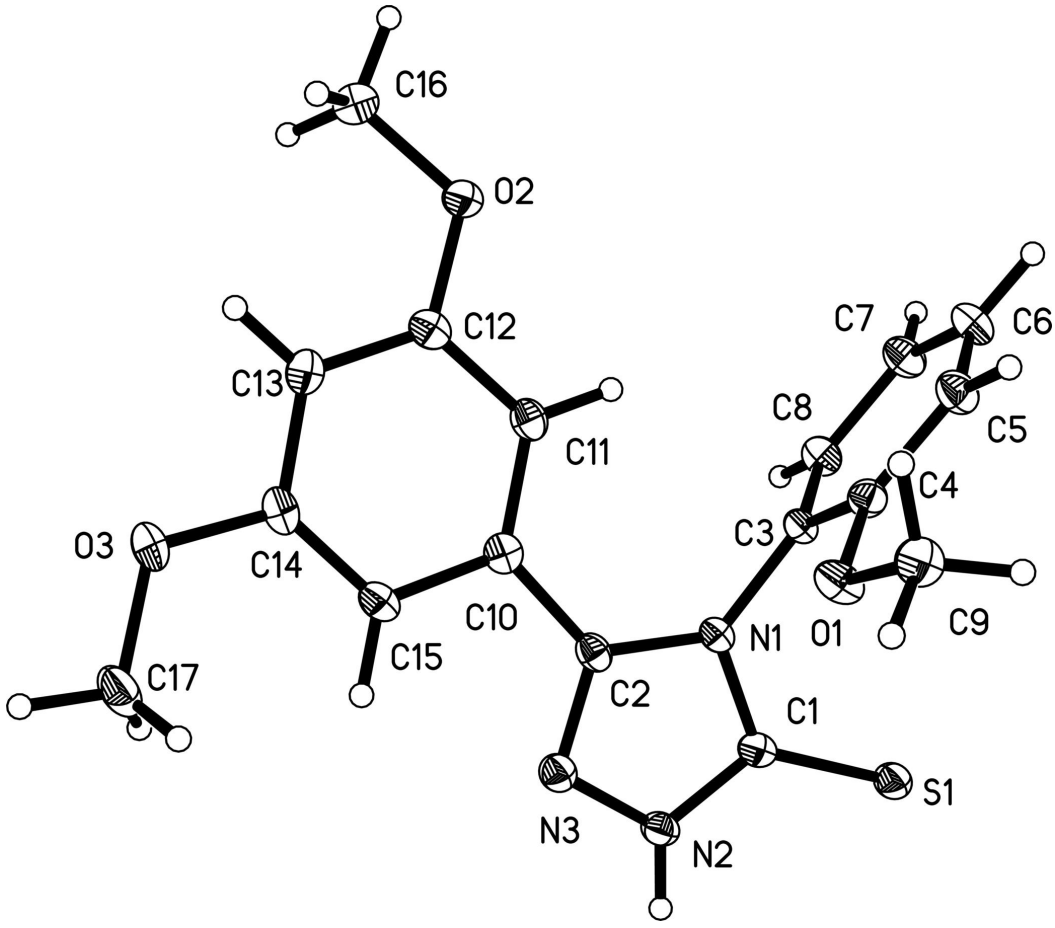

C16
O2
C12
C13
C11
C7
C6
C8
C5
C4
C3
O3
C14
C10
N1
O1
C9
C15
C17
C2
C1
S1
N3
N2

Fig. 2

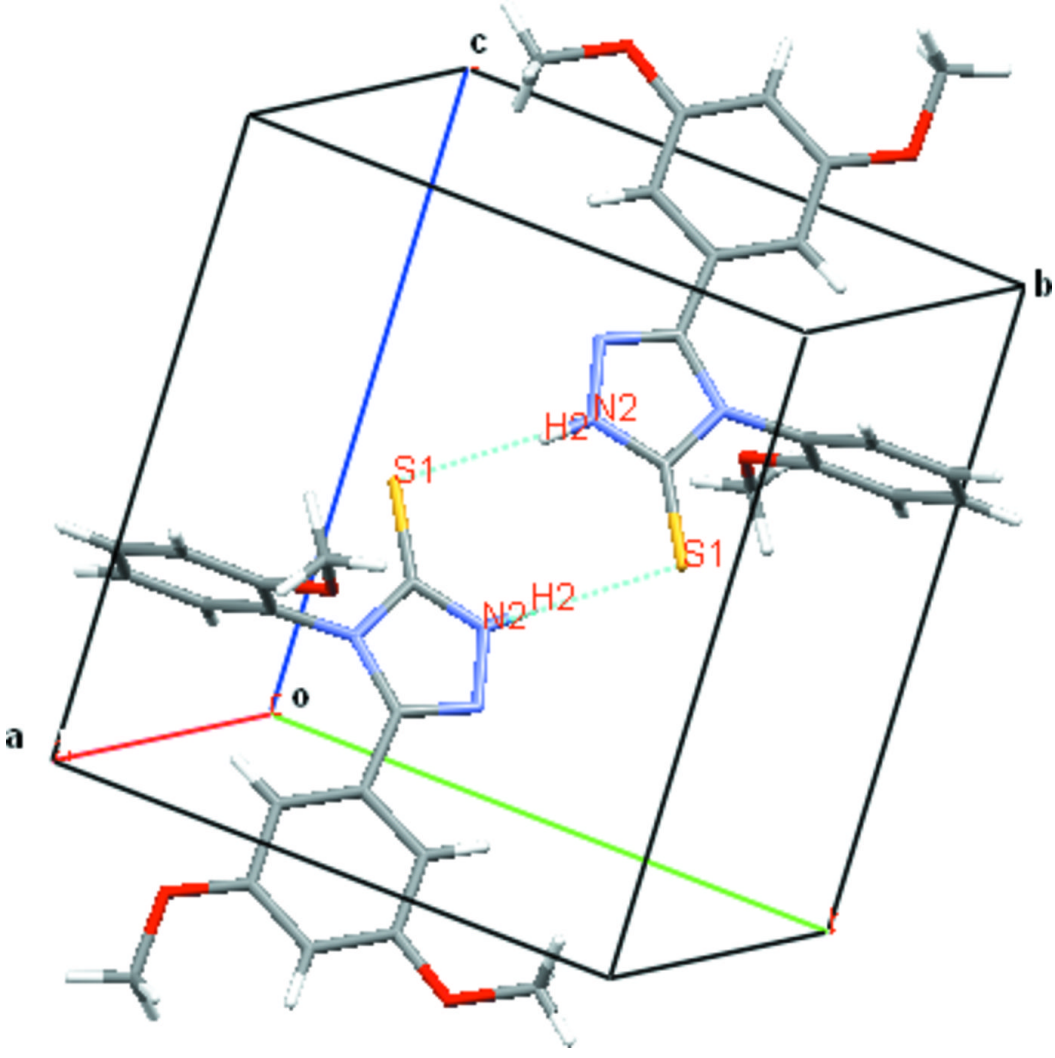
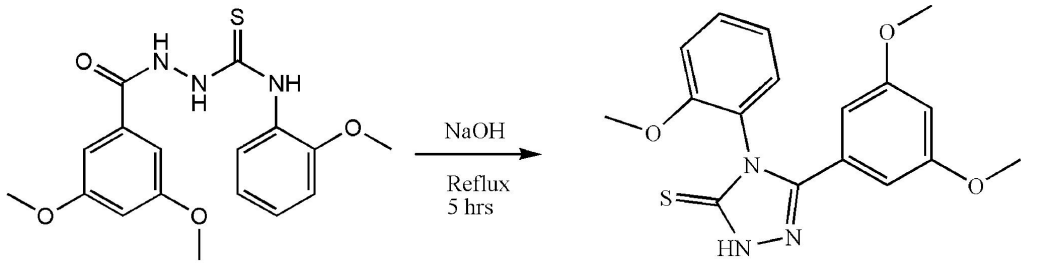


Fig. 3



1-(3,5-dimethoxybenzoyl)-4-(2-methoxy phenyl)thiosemicarbazide

4-(2-methoxyphenyl)-5-(3,5-dimethoxyphenyl) -2H-1,2,4-triazole-3(4H)-thione