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

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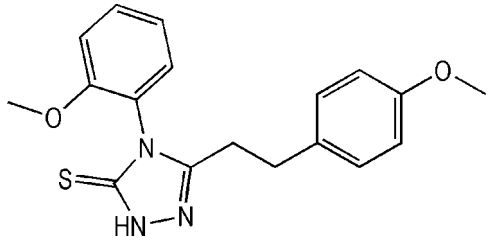
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.002 Å; R factor = 0.034; wR factor = 0.094; data-to-parameter ratio = 14.0.

The title compound, $C_{18}H_{19}N_3O_2S$, 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 82.84 (2) and 78.69 (3)°. In the crystal structure, intermolecular N—H···S and C—H···O hydrogen bonds link the molecules into infinite chains along the *a* axis.

Related literature

For bond-length data, see: Allen *et al.* (1987). For general background, see: Holla *et al.* (1998); Turan-Zitouni *et al.* (1999); Demirbas *et al.* (2002); Paulvannan *et al.* (2000); Kritsanida *et al.* (2002); Omar *et al.* (1986). For related structures, see: Öztürk *et al.* (2004*a*,*b*); Zhang *et al.* (2004).



Experimental

Crystal data

$C_{18}H_{19}N_3O_2S$
M_r = 341.42
Monoclinic, $P2_1/n$
a = 8.3664 (4) Å
b = 19.2172 (10) Å
c = 11.2800 (6) Å
β = 102.133 (1)°
V = 1773.07 (16) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.20 mm^{-1}
T = 298 (2) K
0.38 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD area-dedector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.926, T_{max} = 0.954
8543 measured reflections
3097 independent reflections
2792 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.094
S = 1.03
3097 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···S1^{i}	0.823 (18)	2.468 (18)	3.2864 (14)	173.3 (19)
C6—H6A···O2^{ii}	0.93	2.57	3.278 (2)	133

Symmetry codes: (i) $-x, -y+2, -z+2$; (ii) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

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: HK2292).

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supplementary materials

Acta Cryst. (2007). E**63**, o3502 [**doi:10.1107/S1600536807033867**]

3-(4-Methoxyphenethyl)-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 herein the synthesis and crystal structure of the title compound, (I).

In the molecule of (I) (Fig. 1), the ligand bond lengths and angles are within normal ranges (Allen *et al.*, 1987), and are comparable with those observed in related structures (Öztürk *et al.*, 2004*a*,b). The C1═S1 [1.6782 (15) Å] bond is in accordance with the corresponding values of 1.6773 (19) Å in 4-(4-chlorophenyl)-3-(furan-2-yl)-1*H*-1,2,4-triazole-5(4*H*)-thione (Öztürk *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 N3 ═C9 [1.2997 (19) Å] bond shows double-bond character.

The rings A (N1—N3/C8/C9), B (C1—C6) and C (C12—C17) are, of course, planar and dihedral angles between them are A/B = 82.84 (2)°, A/C = 78.69 (3)° and B/C = 68.63 (3)°.

In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) link the molecules into infinite chains along the *a* axis (Fig. 2), in which they may be effective in the stabilization of the structure.

Experimental

The synthesis of the title compound was carried out by refluxing a solution of 1-(3-(4-methoxyphenyl)propanoyl)-4-(2-methoxyphenyl)thiosemicarbazide (3.41 g, 10 mmol) in 2 *M* NaOH for 5 h. Single crystals suitable for X-ray analysis were obtained by recrystallization from an aqeous ethanol solution at room temperature (yield; 77%; m.p. 459–460 K).

Refinement

H1 (for NH) was located in difference syntheses and refined isotropically [N2—H1 = 0.822 (19) Å and U_{iso}(H) = 0.060 (5) Å^2]. The remaining H atoms were positioned geometrically, with C—H = 0.93, 0.96 and 0.97 Å for aromatic, methylene and methyl H atoms, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

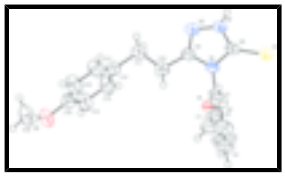


Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

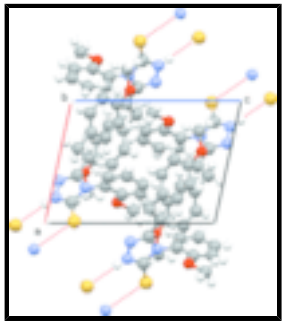


Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

Fig. 3. The reaction scheme for the formation of (I).

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

Crystal data

$C_{18}H_{19}N_3O_2S$	F_{000} = 720
M_r = 341.42	D_x = 1.279 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3874 reflections
a = 8.3664 (4) Å	θ = 2.3–28.3º
b = 19.2172 (10) Å	μ = 0.20 mm^{-1}
c = 11.2800 (6) Å	T = 298 (2) K
β = 102.133 (1)º	Block, colourless
V = 1773.07 (16) Å^3	0.38 × 0.30 × 0.24 mm
Z = 4	

Data collection

Bruker SMART CCD area-dedector diffractometer	3097 independent reflections
Radiation source: fine-focus sealed tube	2792 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.021
T = 298(2) K	θ_{max} = 25.0º
ω and φ scans	θ_{min} = 2.7º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −8→9
T_{min} = 0.926, T_{max} = 0.954	k = −19→22

8543 measured reflections

$l = -13 \rightarrow 13$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.034$

$wR(F^2) = 0.094$

$S = 1.03$

3097 reflections

221 parameters

Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0465P)^2 + 0.4637P]$ where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.002$

$\Delta\rho_{max} = 0.20$ e Å^{-3}

$\Delta\rho_{min} = -0.25$ e Å^{-3}

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 $F^2 > 2\text{sigma}(F^2)$ 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	0.1024 (3)	0.87818 (11)	0.49342 (17)	0.0806 (6)
H1A	0.0592	0.8349	0.5155	0.121*
H1B	0.1865	0.8691	0.4493	0.121*
H1C	0.0164	0.9046	0.4436	0.121*
C2	0.2360 (2)	0.97970 (8)	0.58584 (13)	0.0502 (4)
C3	0.2424 (3)	1.00995 (10)	0.47542 (14)	0.0650 (5)
H3A	0.1980	0.9870	0.4034	0.078*
C4	0.3147 (3)	1.07402 (11)	0.47280 (17)	0.0770 (6)
H4A	0.3154	1.0946	0.3983	0.092*
C5	0.3858 (3)	1.10826 (11)	0.57717 (18)	0.0774 (6)
H5A	0.4378	1.1507	0.5735	0.093*
C6	0.3793 (2)	1.07880 (9)	0.68814 (16)	0.0616 (4)
H6A	0.4261	1.1015	0.7598	0.074*
C7	0.30300 (19)	1.01583 (8)	0.69125 (12)	0.0455 (3)
C8	0.17160 (18)	1.00275 (7)	0.86918 (12)	0.0429 (3)
C9	0.39185 (18)	0.93776 (8)	0.87138 (12)	0.0444 (3)

C10	0.53115 (19)	0.90670 (9)	0.82671 (13)	0.0507 (4)
H10A	0.6131	0.9424	0.8265	0.061*
H10B	0.4924	0.8915	0.7436	0.061*
C11	0.6107 (2)	0.84558 (9)	0.90109 (14)	0.0575 (4)
H11A	0.6605	0.8613	0.9822	0.069*
H11B	0.5280	0.8113	0.9078	0.069*
C12	0.73945 (19)	0.81265 (8)	0.84314 (14)	0.0508 (4)
C13	0.7008 (2)	0.76314 (10)	0.75284 (18)	0.0655 (5)
H13A	0.5933	0.7478	0.7300	0.079*
C14	0.8172 (2)	0.73587 (9)	0.69566 (18)	0.0637 (5)
H14A	0.7877	0.7028	0.6347	0.076*
C15	0.97597 (19)	0.75748 (8)	0.72868 (15)	0.0499 (4)
C16	1.0182 (2)	0.80575 (11)	0.81871 (18)	0.0689 (5)
H16A	1.1261	0.8205	0.8423	0.083*
C17	0.8994 (2)	0.83254 (11)	0.87457 (17)	0.0700 (5)
H17A	0.9296	0.8653	0.9358	0.084*
C18	1.2517 (2)	0.74079 (11)	0.7088 (2)	0.0764 (6)
H18A	1.3127	0.7170	0.6579	0.115*
H18B	1.2852	0.7244	0.7906	0.115*
H18C	1.2716	0.7899	0.7063	0.115*
N1	0.29008 (15)	0.98670 (6)	0.80644 (10)	0.0424 (3)
N2	0.21179 (16)	0.96395 (7)	0.96878 (11)	0.0483 (3)
N3	0.34705 (16)	0.92254 (7)	0.97186 (11)	0.0514 (3)
O1	0.16954 (17)	0.91688 (6)	0.60074 (9)	0.0641 (3)
O2	1.08309 (14)	0.72766 (6)	0.66684 (12)	0.0639 (3)
S1	0.01515 (5)	1.05850 (2)	0.82924 (3)	0.05404 (15)
H1	0.159 (2)	0.9613 (10)	1.0225 (17)	0.060 (5)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.1147 (17)	0.0686 (12)	0.0519 (10)	−0.0098 (11)	0.0023 (10)	−0.0112 (9)
C2	0.0661 (10)	0.0503 (9)	0.0376 (7)	0.0066 (7)	0.0184 (7)	0.0016 (6)
C3	0.0938 (13)	0.0687 (11)	0.0372 (8)	0.0096 (10)	0.0247 (8)	0.0029 (7)
C4	0.1153 (17)	0.0736 (12)	0.0550 (11)	0.0067 (11)	0.0472 (11)	0.0172 (9)
C5	0.1114 (16)	0.0612 (11)	0.0729 (12)	−0.0109 (11)	0.0497 (12)	0.0086 (9)
C6	0.0808 (12)	0.0562 (10)	0.0559 (10)	−0.0072 (8)	0.0326 (9)	−0.0030 (8)
C7	0.0595 (9)	0.0476 (8)	0.0348 (7)	0.0061 (7)	0.0225 (6)	0.0028 (6)
C8	0.0528 (8)	0.0481 (8)	0.0305 (6)	−0.0022 (6)	0.0149 (6)	−0.0057 (6)
C9	0.0506 (8)	0.0486 (8)	0.0357 (7)	0.0002 (6)	0.0134 (6)	−0.0005 (6)
C10	0.0538 (9)	0.0582 (9)	0.0441 (8)	0.0035 (7)	0.0196 (7)	0.0014 (7)
C11	0.0594 (9)	0.0689 (10)	0.0480 (8)	0.0099 (8)	0.0197 (7)	0.0076 (8)
C12	0.0525 (9)	0.0538 (9)	0.0479 (8)	0.0070 (7)	0.0145 (7)	0.0067 (7)
C13	0.0420 (9)	0.0729 (12)	0.0809 (12)	−0.0028 (8)	0.0109 (8)	−0.0134 (9)
C14	0.0503 (9)	0.0643 (10)	0.0754 (11)	−0.0034 (8)	0.0105 (8)	−0.0232 (9)
C15	0.0480 (8)	0.0446 (8)	0.0586 (9)	0.0018 (6)	0.0149 (7)	−0.0021 (7)
C16	0.0475 (9)	0.0762 (12)	0.0842 (13)	−0.0119 (8)	0.0164 (8)	−0.0286 (10)
C17	0.0622 (11)	0.0794 (13)	0.0702 (11)	−0.0087 (9)	0.0175 (9)	−0.0299 (10)

C18	0.0509 (10)	0.0701 (12)	0.1122 (17)	−0.0004 (8)	0.0264 (10)	−0.0164 (11)
N1	0.0529 (7)	0.0470 (7)	0.0310 (5)	0.0019 (5)	0.0168 (5)	−0.0008 (5)
N2	0.0554 (7)	0.0605 (8)	0.0335 (6)	0.0068 (6)	0.0198 (6)	0.0038 (5)
N3	0.0563 (8)	0.0615 (8)	0.0396 (7)	0.0080 (6)	0.0173 (6)	0.0055 (6)
O1	0.0948 (9)	0.0568 (7)	0.0383 (6)	−0.0112 (6)	0.0087 (6)	−0.0009 (5)
O2	0.0504 (6)	0.0600 (7)	0.0851 (8)	−0.0005 (5)	0.0230 (6)	−0.0195 (6)
S1	0.0650 (3)	0.0642 (3)	0.0377 (2)	0.01566 (19)	0.02179 (18)	0.00542 (16)

Geometric parameters (Å, °)

C1—O1	1.431 (2)	C10—H10A	0.9700
C1—H1A	0.9600	C10—H10B	0.9700
C1—H1B	0.9600	C11—C12	1.512 (2)
C1—H1C	0.9600	C11—H11A	0.9700
C2—O1	1.354 (2)	C11—H11B	0.9700
C2—C3	1.386 (2)	C12—C17	1.365 (2)
C2—C7	1.389 (2)	C12—C13	1.382 (2)
C3—C4	1.375 (3)	C13—C14	1.380 (2)
C3—H3A	0.9300	C13—H13A	0.9300
C4—C5	1.371 (3)	C14—C15	1.367 (2)
C4—H4A	0.9300	C14—H14A	0.9300
C5—C6	1.385 (2)	C15—C16	1.366 (2)
C5—H5A	0.9300	C15—O2	1.3715 (19)
C6—C7	1.372 (2)	C16—C17	1.384 (2)
C6—H6A	0.9300	C16—H16A	0.9300
C7—N1	1.4396 (17)	C17—H17A	0.9300
C8—N2	1.3314 (19)	C18—O2	1.413 (2)
C8—N1	1.3687 (18)	C18—H18A	0.9600
C8—S1	1.6782 (15)	C18—H18B	0.9600
C9—N3	1.2997 (19)	C18—H18C	0.9600
C9—N1	1.3726 (19)	N2—N3	1.3777 (18)
C9—C10	1.488 (2)	N2—H1	0.822 (19)
C10—C11	1.514 (2)		
O1—C1—H1A	109.5	C10—C11—H11A	109.5
O1—C1—H1B	109.5	C12—C11—H11B	109.5
H1A—C1—H1B	109.5	C10—C11—H11B	109.5
O1—C1—H1C	109.5	H11A—C11—H11B	108.1
H1A—C1—H1C	109.5	C17—C12—C13	116.71 (15)
H1B—C1—H1C	109.5	C17—C12—C11	121.28 (15)
O1—C2—C3	125.45 (15)	C13—C12—C11	121.96 (15)
O1—C2—C7	116.20 (12)	C14—C13—C12	121.82 (16)
C3—C2—C7	118.35 (16)	C14—C13—H13A	119.1
C4—C3—C2	119.69 (17)	C12—C13—H13A	119.1
C4—C3—H3A	120.2	C15—C14—C13	119.90 (16)
C2—C3—H3A	120.2	C15—C14—H14A	120.1
C5—C4—C3	121.66 (16)	C13—C14—H14A	120.1
C5—C4—H4A	119.2	C16—C15—C14	119.59 (15)
C3—C4—H4A	119.2	C16—C15—O2	124.56 (15)
C4—C5—C6	119.18 (18)	C14—C15—O2	115.85 (14)

C4—C5—H5A	120.4	C15—C16—C17	119.53 (16)
C6—C5—H5A	120.4	C15—C16—H16A	120.2
C7—C6—C5	119.37 (17)	C17—C16—H16A	120.2
C7—C6—H6A	120.3	C12—C17—C16	122.45 (16)
C5—C6—H6A	120.3	C12—C17—H17A	118.8
C6—C7—C2	121.68 (14)	C16—C17—H17A	118.8
C6—C7—N1	119.32 (14)	O2—C18—H18A	109.5
C2—C7—N1	119.00 (13)	O2—C18—H18B	109.5
N2—C8—N1	103.19 (12)	H18A—C18—H18B	109.5
N2—C8—S1	128.94 (11)	O2—C18—H18C	109.5
N1—C8—S1	127.86 (11)	H18A—C18—H18C	109.5
N3—C9—N1	111.06 (13)	H18B—C18—H18C	109.5
N3—C9—C10	126.51 (14)	C8—N1—C9	108.29 (11)
N1—C9—C10	122.42 (12)	C8—N1—C7	125.38 (12)
C9—C10—C11	114.06 (12)	C9—N1—C7	126.32 (12)
C9—C10—H10A	108.7	C8—N2—N3	113.90 (12)
C11—C10—H10A	108.7	C8—N2—H1	125.3 (13)
C9—C10—H10B	108.7	N3—N2—H1	120.6 (13)
C11—C10—H10B	108.7	C9—N3—N2	103.53 (12)
H10A—C10—H10B	107.6	C2—O1—C1	117.17 (13)
C12—C11—C10	110.81 (13)	C15—O2—C18	117.90 (14)
C12—C11—H11A	109.5		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H1···S1^{i}	0.823 (18)	2.468 (18)	3.2864 (14)	173.3 (19)
C6—H6A···O2^{ii}	0.93	2.57	3.278 (2)	133

Symmetry codes: (i) −*x*, −*y*+2, −*z*+2; (ii) −*x*+3/2, *y*+1/2, −*z*+3/2.

Fig. 1

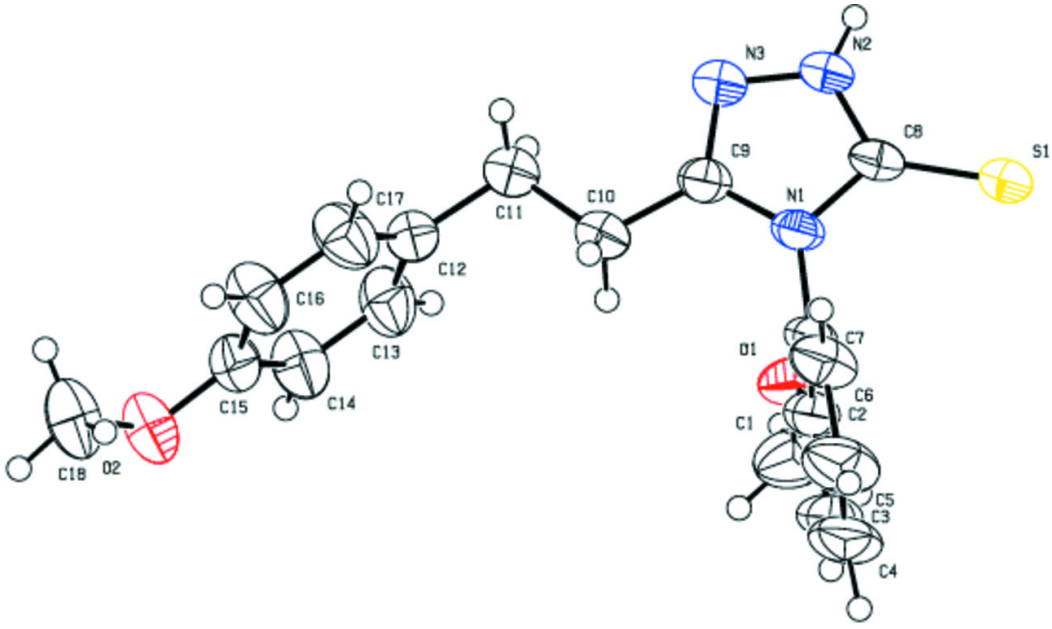

N3
N2
C8
S1
C9
C17
C11
C10
N1
C12
C16
C13
O1
C7
C6
C2
C1
C15
C14
C5
C3
C18
O2
C4

Fig. 2

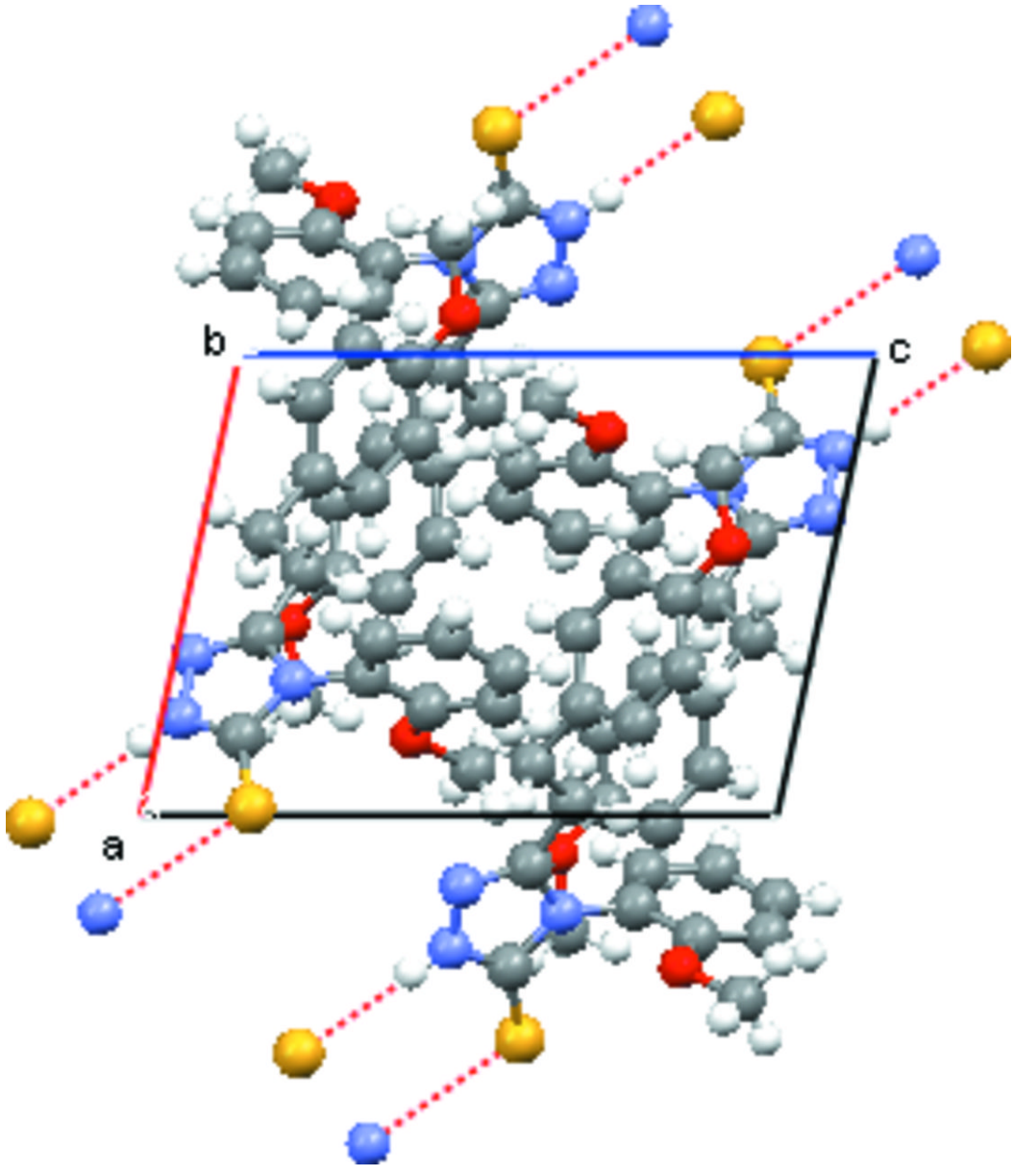
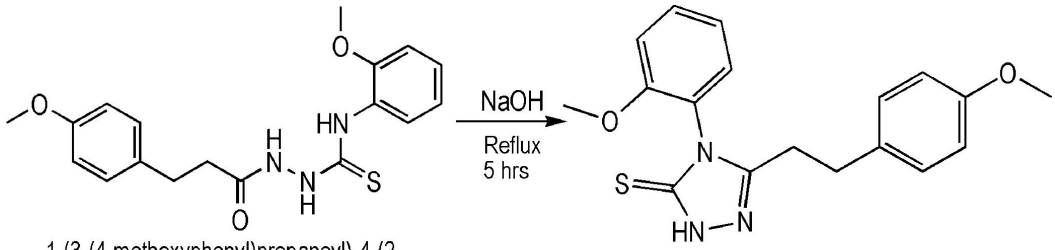


Fig. 3



1-(3-(4-methoxyphenyl)propanoyl)-4-(2-methoxyphenyl)thiosemicarbazide

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