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4-Amino-3-{5-[(3,5-dimethyl-1*H*-pyrazol-1-yl)carbonyl]-2,6-dimethyl-3-pyridyl}-1*H*-1,2,4-triazole-5(4*H*)-thione

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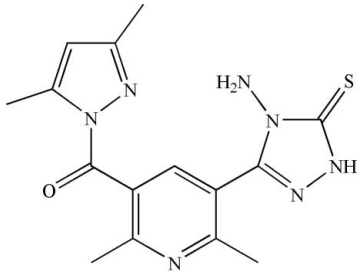
Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.051; wR factor = 0.136; data-to-parameter ratio = 12.9.

The title compound, $C_{15}H_{17}N_7OS$, is a new heterocyclic compound and this is the first time its synthesis has been reported. The compound, which contains a 1,2,4-triazole ring, a pyridine ring and a pyrazole ring, has potential biological activity and pharmacological properties. Molecules are linked by intermolecular N—H···N hydrogen bonds.

Related literature

For general background, see: Soliman & Darwish (1983); Holla & Kalluraya (1988); Prasad *et al.* (1989); Elwahy & Abbas (2000); Pandeya *et al.* (2000); Soudi *et al.* (2005); Tardito *et al.* (2007). For related literature, see: Özbey *et al.* (2000); Bruno *et al.* (2003); Xue *et al.* (2004); Yang & Liu (2005).



Experimental

Crystal data

$C_{15}H_{17}N_7OS$
M_r = 343.42
Triclinic, $P\overline{1}$
a = 8.039 (5) Å
b = 8.428 (5) Å
c = 12.391 (8) Å
α = 102.186 (7)°
β = 90.633 (8)°
γ = 90.074 (8)°
V = 820.5 (9) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 273 (2) K
0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.968
4304 measured reflections
2861 independent reflections
2142 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.136
S = 1.03
2861 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···N7^{i}	0.86	2.11	2.873 (3)	148

Symmetry code: (i) $-x, -y+2, -z$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

The authors thank the Instrument Analysis and Research Center of Shanghai University for the X-ray diffraction data analysis.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WK2068).

References

Bruker (2000). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2005). *APEX2*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruno, G., Nicoló, F., Puntoriero, F., Giuffrida, G., Ricevuto, V. & Rosace, G. (2003). *Acta Cryst.* C**59**, o390–o391.
Elwahy, A. H. & Abbas, A. A. (2000). *Tetrahedron*, **56**, 885–895.
Holla, B. S. & Kalluraya, B. (1988). *Indian J. Chem. Sect. B*, **27**, 683–685.
Özbey, S., Ulusoy, N. & Kendi, E. (2000). *Acta Cryst.* C**56**, 222–224.
Pandeya, S. N., Sriram, D., Nath, G. & De, C. E. (2000). *Arzneim. Forsch.* **50**, 55–59.
Prasad, A. R., Ramalingam, T., Rao, A. B., Diwan, P. W. & Sattur, P. B. (1989). *Eur. J. Med. Chem.* **24**, 199–201.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Soliman, R. & Darwish, S. A. (1983). *J. Med. Chem.* **26**, 1659–1663.
Soudi, A. A., Marandi, F., Morsali, A., Kempe, R. & Hertle, I. (2005). *J. Coord. Chem.* **58**, 1631–1637.
Tardito, S., Bussolati, O., Maffini, M., Tegoni, M., Giannetto, M., Dall'Asta, V., Franchi, G. R., Lanfranchi, M., Pellinghelli, M. A., Mucchino, C., Mori, G. & Marchio, L. (2007). *J. Med. Chem.* **50**, 1916–1924.
Xue, S. J., Duan, L. P., Ke, S. Y. & Zhu, J. M. (2004). *Chin. J. Struct. Chem.* **23**, 441–444.
Yang, L.-M. & Liu, Z.-J. (2005). *Acta Cryst.* E**61**, o1466–o1468.

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supplementary materials

Acta Cryst. (2007). E**63**, o3846 [**doi:10.1107/S1600536807038640**]

4-Amino-3-{5-[(3,5-dimethyl-1*H*-pyrazol-1-yl)carbonyl]-2,6-dimethyl-3-pyridyl}-1*H*-1,2,4-triazole-5(4*H*)-thione

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Comment

Nitrogen-containing heterocycles compounds are well known natural products moieties which represent interesting biological activities and pharmacological properties (Pandeya *et al.*, 2000; Soudi *et al.*, 2005). For example, the 1,2,4-triazole nucleus with the nitrogen-bridged heterocycles always show antibacterial (Holla & Kalluraya, 1988) and antifungal (Prasad *et al.*, 1989) properties. In addition, the substituted 1,2,4-triazol is a well established N-donor heterocyclic ligand (Elwahy & Abbas, 2000). More recently, it was reported that 1,2,4-triazole derivatives complexed with metal have higher biological activity (Tardito *et al.*, 2007). Further more, the substituted 3,5-Dimethylpyrazoles contribute significant activities to diabetes (Soliman & Darwish,1983). These useful applications for the important class of nitrogen-containing heterocycles attracted our attention. Here, we report the synthesis and structure of a new multi-heterocyclic compound.

In the molecule of the title compound, (I), (Fig. 1), the C1—N2, C2—N3 bond distances [average =1.317 (3) Å] and N2—N3 bond distance [1.369 (3) Å] are in good agreement with those found for structures containing the 1,2,4-trizole ring Özbey *et al.*, 2000; Bruno *et al.*, 2003). The C=S double bond [1.663 (3) Å] is equal to the corresponding double bond (Xue *et al.*, 2004). In the pyrazole ring, the bond distances between atoms are similar with those in the literature (Yang & Liu, 2005).

It is interesting to find that the three rings are not coplanar, due to steric hinderance. The angle between triazole plane and pyridine plane is 28.90 (3)°, whereas the angle between pyrazole plane and pyridine plane is 53.26 (9)°. Furthermore, the planes of triazole and pyrazole form a dihedral angle 55.55 (2)°. As a result of the torsional angle of the title compound, the steric hinderance has been reduced that make the compound more stable.

Experimental

The synthetic route is depicted in Scheme 1. For the synthesis of I, 5-carbethoxy-2,6-dimethylpyridine-3-carboxhydrazide (0.47 g, 2 mmol) was dissolved in anhydrous ethanol(5 ml) in the presence of carbon bisulfide (0.23 g, 3 mmol) and potassium hydroxide (0.17 g, 3 mmol). The mixture was stirred at room temperature for 4 h. After removal of the solvent, hydrazine hydrate was added as solvent, heated and stirred under reflux for 3 h. After cooling to room temperature, the mixture was neutralized with dilute hydrochloric acid. The precipitate formed was filtered and washed with water. A colorless solid was obtained and directly used for next step without further purification. The obtained product (0.28 g, 1 mmol) and acetylacetone (0.1 g, 1 mmol) were put together in chloroform (5 ml) with hydrochloric acid as catalyst. The mixture was heated to reflux for 3 h, cooled to room temperature and then solvent removed. The crude product was filtered, washed with water and dried. It was recrystallized from ethanol to give a colorless compound in a yield of 76% (m. p. 414 K– 415 K). IR(ν, cm^{-1}): 3302 (NH), 3097 (pyridine CH), 2925 (CH), 1699 (C=O), 1603–1481 (C=C, C=N), 1338 (C=S); ^{1}H-NMR (500 MHz, DMSO-d_6): δ 14.03 (s, 1H, triazole NH), 8.06 (s, 1H, pyridine CH), 6.32 (s, 1H, pyrazole CH), 5.60 (s, 1H, triazole NH), 2.60 (s, 3H, pyridine CH), 2.53 (s, 3H, pyridine CH), 2.39 (s, 3H, pyrazole CH), 2.11(s, 3H, pyrazole CH); Elemental analysis, required

for $C_{15}H_{17}N_7OS$: C 52.46, H 4.99, N 28.55%; Found: C 52.33, H 4.87, N 28.65%. Single crystals suitable for X-ray analysis were obtained from ethanol by slow evaporation at room temperature.

Refinement

All H atoms were placed in calculated positions, with C—H=0.93–0.96 Å; N—H=0.86 Å, and included in the final cycles of refinement using a riding model,U_{iso}(H) = 1.2U_{eq}(C).

Figures

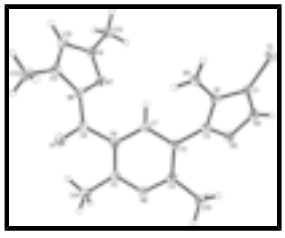

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

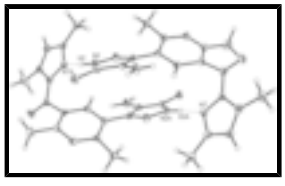

Fig. 2. Diagram showing hydrogen bonding for (I). Hydrogen bonds are shown as dashed lines.

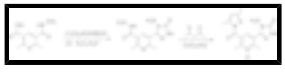

Fig. 3. The formation of the title compound.

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Crystal data

$C_{15}H_{17}N_7OS$	Z = 2
M_r = 343.42	F_{000} = 360
Triclinic, $P\overline{1}$	D_x = 1.390 Mg m^{-3}
a = 8.039 (5) Å	Mo $K\alpha$ radiation λ = 0.71073 Å
b = 8.428 (5) Å	Cell parameters from 1268 reflections
c = 12.391 (8) Å	θ = 2.7–23.5º
α = 102.186 (7)º	μ = 0.22 mm^{-1}
β = 90.633 (8)º	T = 273 (2) K
γ = 90.074 (8)º	Block, colorless
V = 820.5 (9) Å^3	0.20 × 0.20 × 0.15 mm

Data collection

Bruker APEX II CCD area-detector diffractometer	2861 independent reflections
Radiation source: fine-focus sealed tube	2142 reflections with $I > 2\sigma(I)$

Monochromator: graphite
T = 273(2) K
φ and ω scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.968
4304 measured reflections

R_{int} = 0.018
θ_{max} = 25.1º
θ_{min} = 2.5º
h = −6→9
k = −10→9
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.136
S = 1.03
2861 reflections
222 parameters
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0567P)^2 + 0.5239P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.45 e Å^{-3}
Extinction correction: SHELXL97, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.004 (3)

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 basedon 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}
S1	0.43077 (10)	0.93706 (11)	−0.18895 (7)	0.0538 (3)
C1	0.2477 (4)	0.8830 (3)	−0.1465 (2)	0.0384 (6)
C2	0.0464 (3)	0.7909 (3)	−0.0528 (2)	0.0351 (6)
C3	−0.0417 (3)	0.7246 (3)	0.0307 (2)	0.0348 (6)
C4	−0.1962 (3)	0.6475 (3)	0.0077 (2)	0.0369 (6)
C5	−0.2259 (4)	0.6266 (3)	0.1905 (2)	0.0424 (7)
C6	−0.0675 (3)	0.6903 (3)	0.2172 (2)	0.0369 (6)
C7	0.0229 (3)	0.7418 (3)	0.1367 (2)	0.0364 (6)
H7	0.1275	0.7882	0.1537	0.044*

C8	0.0107 (3)	0.6855 (4)	0.3260 (2)	0.0410 (7)
C9	0.1963 (3)	1.0647 (4)	0.4101 (2)	0.0427 (7)
C10	0.2723 (4)	0.9843 (4)	0.4868 (2)	0.0470 (7)
H10	0.3484	1.0294	0.5418	0.056*
C11	0.2150 (4)	0.8312 (4)	0.4659 (2)	0.0444 (7)
C12	0.2215 (4)	1.2347 (4)	0.3972 (3)	0.0566 (9)
H12A	0.1676	1.2492	0.3305	0.085*
H12B	0.3384	1.2562	0.3935	0.085*
H12C	0.1749	1.3083	0.4592	0.085*
C13	0.2588 (5)	0.6943 (4)	0.5193 (3)	0.0661 (10)
H13A	0.3405	0.7300	0.5764	0.099*
H13B	0.3031	0.6065	0.4651	0.099*
H13C	0.1609	0.6581	0.5509	0.099*
C14	−0.3432 (4)	0.5825 (5)	0.2724 (3)	0.0671 (10)
H14A	−0.4510	0.6267	0.2629	0.101*
H14B	−0.3025	0.6259	0.3459	0.101*
H14C	−0.3513	0.4664	0.2611	0.101*
C15	−0.2747 (4)	0.6067 (4)	−0.1048 (2)	0.0465 (7)
H15A	−0.3550	0.5214	−0.1076	0.070*
H15B	−0.1906	0.5714	−0.1588	0.070*
H15C	−0.3291	0.7010	−0.1201	0.070*
N1	0.2156 (3)	0.8125 (3)	−0.05885 (17)	0.0360 (5)
N2	0.0964 (3)	0.8979 (3)	−0.18831 (19)	0.0436 (6)
H2	0.0793	0.9383	−0.2456	0.052*
N3	−0.0292 (3)	0.8433 (3)	−0.13175 (19)	0.0433 (6)
N4	0.3343 (3)	0.7712 (3)	0.01276 (19)	0.0471 (7)
H4A	0.4379	0.7897	0.0038	0.057*
H4B	0.3041	0.7271	0.0661	0.057*
N5	−0.2849 (3)	0.6039 (3)	0.08698 (19)	0.0425 (6)
N6	0.1045 (3)	0.8203 (3)	0.37803 (17)	0.0382 (6)
N7	0.0934 (3)	0.9668 (3)	0.34468 (18)	0.0394 (6)
O1	−0.0008 (3)	0.5692 (3)	0.36724 (18)	0.0606 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0503 (5)	0.0658 (6)	0.0487 (5)	−0.0140 (4)	0.0003 (4)	0.0197 (4)
C1	0.0490 (17)	0.0332 (15)	0.0329 (14)	−0.0039 (12)	−0.0013 (12)	0.0069 (11)
C2	0.0382 (15)	0.0368 (15)	0.0301 (13)	0.0014 (12)	−0.0031 (11)	0.0064 (11)
C3	0.0357 (14)	0.0340 (15)	0.0346 (14)	0.0017 (11)	−0.0029 (11)	0.0071 (11)
C4	0.0384 (15)	0.0350 (15)	0.0367 (14)	0.0014 (12)	−0.0046 (12)	0.0063 (12)
C5	0.0469 (17)	0.0422 (17)	0.0374 (15)	−0.0078 (13)	−0.0011 (13)	0.0066 (12)
C6	0.0413 (15)	0.0354 (15)	0.0337 (14)	−0.0041 (12)	−0.0037 (12)	0.0067 (12)
C7	0.0350 (15)	0.0350 (15)	0.0382 (15)	−0.0017 (11)	−0.0029 (12)	0.0056 (12)
C8	0.0424 (16)	0.0458 (17)	0.0355 (15)	−0.0056 (13)	−0.0022 (12)	0.0102 (13)
C9	0.0418 (16)	0.0470 (17)	0.0372 (15)	−0.0033 (13)	0.0004 (13)	0.0045 (13)
C10	0.0452 (17)	0.0539 (19)	0.0400 (16)	−0.0069 (14)	−0.0110 (13)	0.0062 (14)
C11	0.0431 (17)	0.0540 (19)	0.0372 (15)	−0.0027 (14)	−0.0064 (13)	0.0121 (14)

C12	0.070 (2)	0.0453 (19)	0.0527 (19)	−0.0090 (16)	−0.0065 (16)	0.0070 (15)
C13	0.073 (2)	0.070 (2)	0.062 (2)	−0.0075 (19)	−0.0284 (18)	0.0305 (18)
C14	0.059 (2)	0.094 (3)	0.0483 (19)	−0.032 (2)	−0.0001 (16)	0.0162 (19)
C15	0.0461 (17)	0.0526 (19)	0.0397 (16)	−0.0055 (14)	−0.0110 (13)	0.0077 (14)
N1	0.0368 (13)	0.0366 (13)	0.0350 (12)	−0.0020 (10)	−0.0022 (10)	0.0082 (10)
N2	0.0469 (14)	0.0512 (15)	0.0368 (13)	−0.0003 (11)	−0.0021 (11)	0.0186 (11)
N3	0.0403 (13)	0.0511 (15)	0.0415 (13)	0.0020 (11)	−0.0001 (11)	0.0167 (11)
N4	0.0328 (13)	0.0736 (18)	0.0436 (14)	−0.0076 (12)	−0.0081 (10)	0.0323 (13)
N5	0.0396 (13)	0.0462 (15)	0.0405 (13)	−0.0066 (11)	−0.0042 (10)	0.0068 (11)
N6	0.0417 (13)	0.0418 (14)	0.0324 (12)	−0.0034 (10)	−0.0047 (10)	0.0106 (10)
N7	0.0439 (14)	0.0383 (13)	0.0370 (12)	−0.0008 (10)	−0.0027 (10)	0.0106 (10)
O1	0.0802 (17)	0.0545 (14)	0.0542 (13)	−0.0188 (12)	−0.0156 (12)	0.0284 (11)

Geometric parameters (Å, °)

S1—C1	1.663 (3)	C10—H10	0.9300
C1—N2	1.333 (4)	C11—N6	1.385 (3)
C1—N1	1.370 (3)	C11—C13	1.487 (4)
C2—N3	1.301 (3)	C12—H12A	0.9600
C2—N1	1.377 (3)	C12—H12B	0.9600
C2—C3	1.463 (4)	C12—H12C	0.9600
C3—C7	1.386 (4)	C13—H13A	0.9600
C3—C4	1.400 (4)	C13—H13B	0.9600
C4—N5	1.333 (4)	C13—H13C	0.9600
C4—C15	1.495 (4)	C14—H14A	0.9600
C5—N5	1.338 (4)	C14—H14B	0.9600
C5—C6	1.390 (4)	C14—H14C	0.9600
C5—C14	1.496 (4)	C15—H15A	0.9600
C6—C7	1.382 (4)	C15—H15B	0.9600
C6—C8	1.490 (4)	C15—H15C	0.9600
C7—H7	0.9300	N1—N4	1.390 (3)
C8—O1	1.201 (3)	N2—N3	1.369 (3)
C8—N6	1.398 (4)	N2—H2	0.8600
C9—N7	1.313 (3)	N4—H4A	0.8600
C9—C10	1.412 (4)	N4—H4B	0.8600
C9—C12	1.489 (4)	N6—N7	1.385 (3)
C10—C11	1.341 (4)		
N2—C1—N1	102.8 (2)	C9—C12—H12C	109.5
N2—C1—S1	129.0 (2)	H12A—C12—H12C	109.5
N1—C1—S1	128.2 (2)	H12B—C12—H12C	109.5
N3—C2—N1	110.1 (2)	C11—C13—H13A	109.5
N3—C2—C3	123.1 (2)	C11—C13—H13B	109.5
N1—C2—C3	126.8 (2)	H13A—C13—H13B	109.5
C7—C3—C4	117.8 (2)	C11—C13—H13C	109.5
C7—C3—C2	120.8 (2)	H13A—C13—H13C	109.5
C4—C3—C2	121.4 (2)	H13B—C13—H13C	109.5
N5—C4—C3	121.3 (2)	C5—C14—H14A	109.5
N5—C4—C15	114.7 (2)	C5—C14—H14B	109.5
C3—C4—C15	124.0 (2)	H14A—C14—H14B	109.5

N5—C5—C6	120.8 (3)	C5—C14—H14C	109.5
N5—C5—C14	115.2 (3)	H14A—C14—H14C	109.5
C6—C5—C14	124.0 (3)	H14B—C14—H14C	109.5
C7—C6—C5	118.7 (2)	C4—C15—H15A	109.5
C7—C6—C8	120.4 (2)	C4—C15—H15B	109.5
C5—C6—C8	120.6 (2)	H15A—C15—H15B	109.5
C6—C7—C3	120.2 (3)	C4—C15—H15C	109.5
C6—C7—H7	119.9	H15A—C15—H15C	109.5
C3—C7—H7	119.9	H15B—C15—H15C	109.5
O1—C8—N6	120.2 (3)	C1—N1—C2	108.8 (2)
O1—C8—C6	122.2 (3)	C1—N1—N4	125.6 (2)
N6—C8—C6	117.5 (2)	C2—N1—N4	125.7 (2)
N7—C9—C10	110.6 (3)	C1—N2—N3	114.0 (2)
N7—C9—C12	120.8 (3)	C1—N2—H2	123.0
C10—C9—C12	128.6 (3)	N3—N2—H2	123.0
C11—C10—C9	107.7 (3)	C2—N3—N2	104.4 (2)
C11—C10—H10	126.1	N1—N4—H4A	120.0
C9—C10—H10	126.1	N1—N4—H4B	120.0
C10—C11—N6	105.6 (3)	H4A—N4—H4B	120.0
C10—C11—C13	129.8 (3)	C4—N5—C5	120.9 (2)
N6—C11—C13	124.6 (3)	C11—N6—N7	111.0 (2)
C9—C12—H12A	109.5	C11—N6—C8	127.8 (2)
C9—C12—H12B	109.5	N7—N6—C8	121.2 (2)
H12A—C12—H12B	109.5	C9—N7—N6	105.1 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···N7^{i}	0.86	2.11	2.873 (3)	148

Symmetry codes: (i) −*x*, −*y*+2, −*z*.

Fig. 1

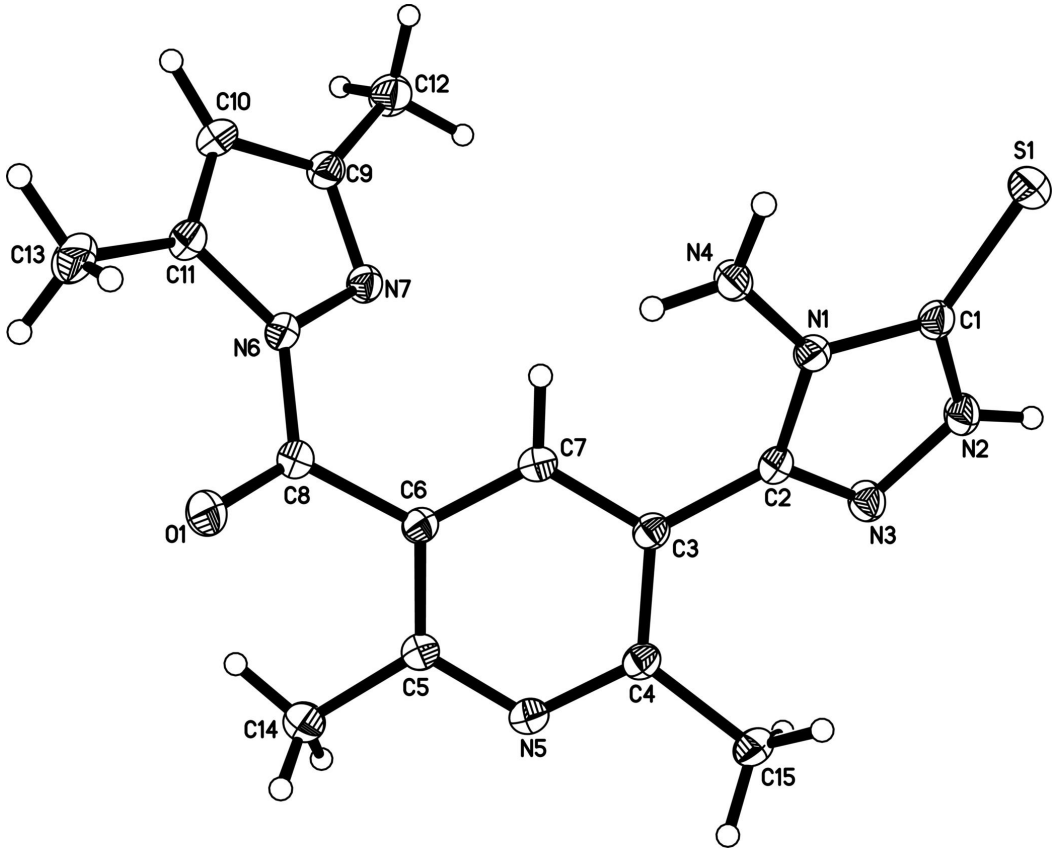

C10
C12
C9
S1
C13
C11
N7
N4
N1
C1
N6
C7
N2
C8
C6
C2
O1
N3
C3
C5
C4
C14
N5
C15

Fig. 2

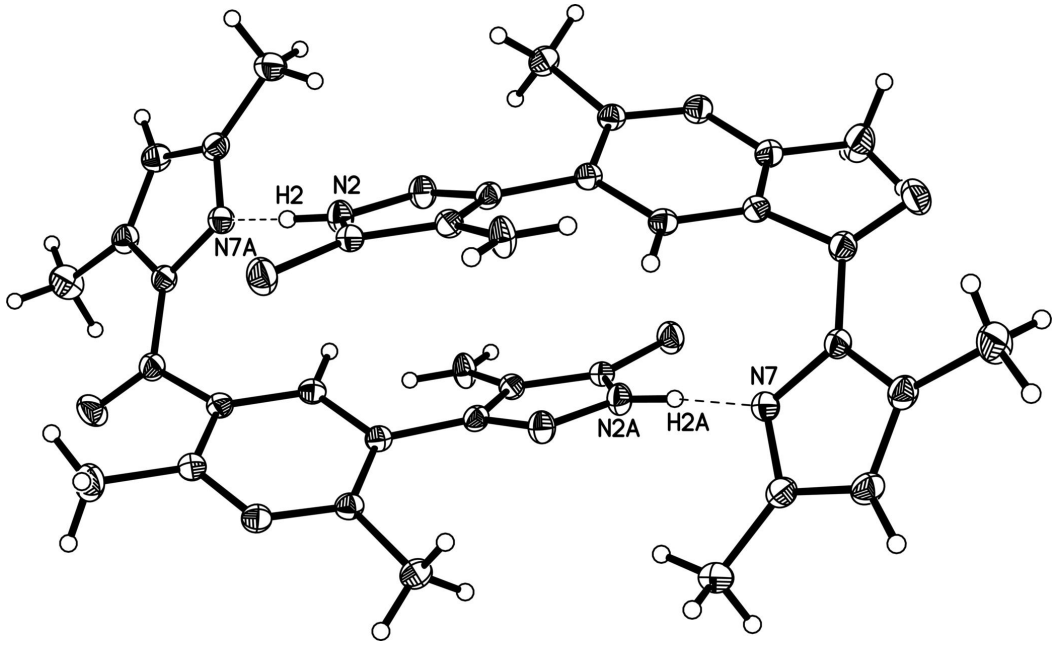
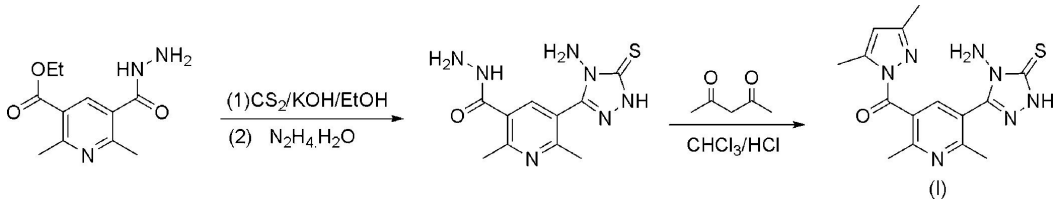


Fig. 3


OEt
HN
NH2
O
O
N
(1)CS2/KOH/EtOH
(2) N2H4.H2O
H2N
NH
O
N
H2N
N
S
N
NH
O
CHCl3/HCl
(I)