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6-(4-Methoxyphenyl)-3-phenyl-1,2,4,5-tetrazine

Feng Xu and Wei-Xiao Hu*

College of Pharmaceutical Science, Zhejiang University of Technology, Hangzhou 310032, People's Republic of China

Correspondence e-mail: huyang@mail.hz.zj.cn

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In the title molecule, $C_{16}H_{14}N_4O$, the tetrazine ring makes dihedral angles of 6.77 (12) and 70.5 (5)° with the phenyl and methoxy-substituted benzene rings, respectively. The crystal packing exhibits π–π stacking interactions and weak intermolecular C—H···N hydrogen bonds.

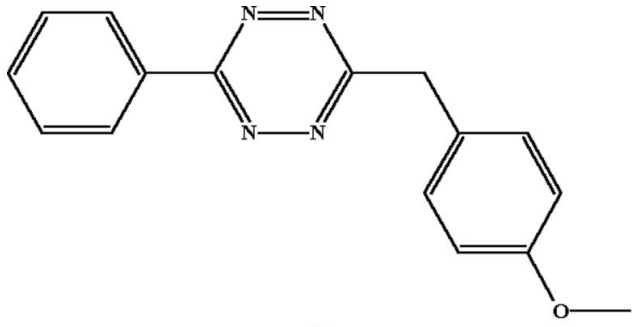
Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.064
wR factor = 0.167
Data-to-parameter ratio = 16.1

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

1,2,4,5-Tetrazine derivatives have high potential for biological activity, possessing a wide spectrum of antiviral and antitumor properties. They have been widely used in pesticides and herbicides (Sauer, 1996). In our search for structure–activity relationships in 1,2,4,5-tetrazine derivatives (Hu *et al.*, 2004, 2005), we obtained red crystals of the title compound, (I).



(I)

In (I) (Fig. 1), the tetrazine ring (centroid *Cg*1) makes dihedral angles of 70.5 (5) and 6.77 (12)° with the aromatic rings C8–C13 (centroid *Cg*2) and C14–C19 (centroid *Cg*3), respectively. The crystal packing exhibits weak intermolecular C—H···N hydrogen-bonding (Table 1) and π–π stacking interactions [indicated by the short distances $Cg1\cdots Cg2^{ii}$ = 3.694 (3) and $Cg1\cdots Cg3^{iii}$ = 3.715 (2) Å; symmetry codes: (ii) $-x, -y, 1-z$; (iii) $1-x, \frac{1}{2}-y, \frac{3}{2}-z$].

Experimental

With sulfur (1.0 g) as catalyst, 85% hydrazine hydrate (10 ml, 170 mmol) was dropped into a mixed anhydrous ethanol (15 ml) solution of 4-methoxybenzyl cyanide (50 mmol) and benzonitrile (50 mmol) at 295 K. After refluxing for 3 h, the mixture was cooled to room temperature and the resulting solid product was filtered off. It was dissolved in diethyl ether (15 ml), and oxidized by sodium nitrate (14 mmol) and acetic acid (14 mmol) for 2 h to afford the product, which was purified by preparative thin-layer chromatography over silica-gel PF254 (2 mm) (cyclohexane–dichloromethane, 1:1) to give red single crystals. X-ray quality single crystals of (I) were obtained by slow evaporation at room temperature of a tetrahydrofuran–anhydrous ethanol (4:1 *v*/*v*) solution.

Crystal data

$C_{16}H_{14}N_4O$
M_r = 278.31
Monoclinic, $P2_1/c$
a = 8.599 (4) Å
b = 15.255 (6) Å
c = 11.794 (4) Å
β = 112.67 (2)°
V = 1427.5 (9) Å^3
Z = 4
D_x = 1.295 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, red
0.30 × 0.25 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.975, T_{max} = 0.983
6907 measured reflections
3083 independent reflections
1923 reflections with $I > 2\sigma(I)$
R_{int} = 0.062
θ_{max} = 27.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.167
S = 1.00
3083 reflections
192 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0862P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.160 (10)

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···N5^{i}	0.93	2.56	3.413 (2)	152

Symmetry code: (i) $x, -y+\frac{1}{2}, z-\frac{1}{2}$.

Methyl H atoms were placed in calculated positions, with C—H = 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C). Other H atoms were placed in calculated positions, with C—H = 0.93–0.97 Å, and refined in riding mode, with U_{iso}(H) = 1.2U_{eq}(C).

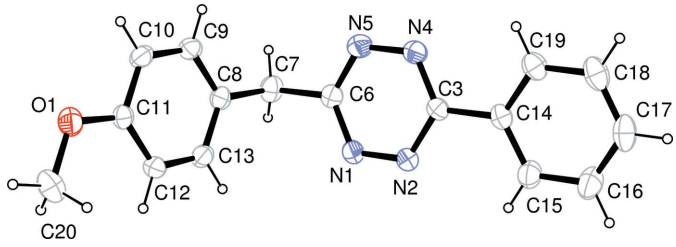


Figure 1
The molecular structure of (I), shown with 30% probability displacement ellipsoids (arbitrary spheres for H atoms).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999); software used to prepare material for publication: *SHELXL97*.

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