

Feng Xu, Wei-Xiao Hu,* Wei
Zhou and Chun-Nian XiaCollege of Pharmaceutical Science, Zhejiang
University of Technology, Hangzhou 310032,
People's Republic of China

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

Key indicators

Single-crystal X-ray study
 $T = 293\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.009\text{ \AA}$
 R factor = 0.076
 wR factor = 0.202
Data-to-parameter ratio = 7.9For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

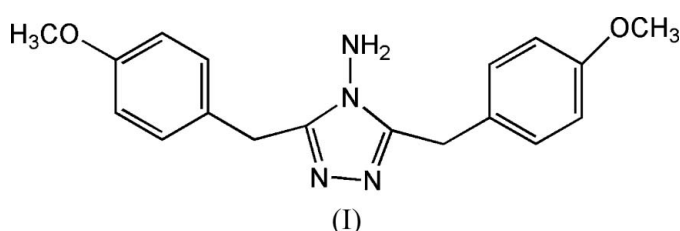
1-Amino-2,5-bis(4-methoxybenzyl)-1,3,4-triazole

In the title compound, $\text{C}_{18}\text{H}_{20}\text{N}_4\text{O}_2$, the triazole ring is twisted with respect to the two benzene rings with dihedral angles of $71.5(3)$ and $67.3(3)^\circ$. $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonding occurs between neighboring molecules.

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Comment

1,3,4-Triazole derivatives have extensive biological activity, including antibacterial and herbicidal action *via* effects on DNA and related molecules (Kahn & Martinez, 1998). Antiviral properties have also been found for some derivatives of 1-amino-1,3,4-triazole-ribofuranoside (Zakharieva *et al.*, 1994). We recently obtained the title triazole compound, (I), during the preparation of *s*-tetrazine derivatives.



The molecular structure of (I) is illustrated in Fig. 1. The molecule has a pseudo-twofold axis. The triazole ring plane is twisted with respect to the benzene rings, the dihedral angles being $71.5(3)$ ($\text{C}8$ -benzene ring) and $67.3(3)^\circ$ ($\text{C}16$ -benzene ring). $\text{N}-\text{H}\cdots\text{N}$ hydrogen bonding occurs between neighboring molecules (Table 1).

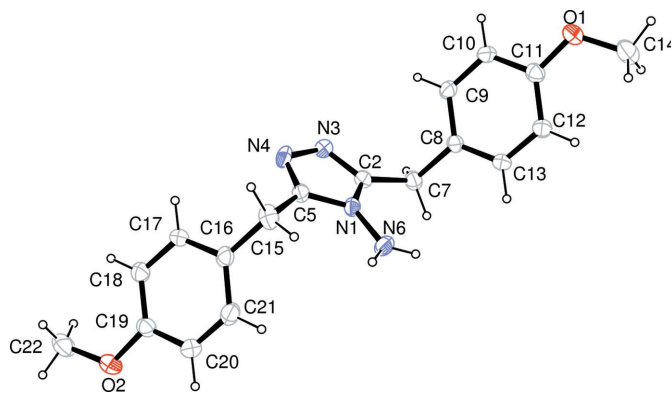


Figure 1

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

Experimental

With sulfur (1.0 g) as a catalyst, 85% hydrazine hydrate (10 ml, 170 mmol) was dropped into *p*-methoxybenzyl cyanide (50 mmol) in anhydrous ethanol (15 ml) at 295 K. After refluxing for 3 h, the mixture was cooled to room temperature and the resulting solid product was filtered off. The solid product was dissolved in dichloromethane, affording single crystals of (I) by evaporation.

Crystal data

| | |
|---------------------------------|---|
| $C_{18}H_{20}N_4O_2$ | $Z = 4$ |
| $M_r = 324.38$ | $D_x = 1.276 \text{ Mg m}^{-3}$ |
| Monoclinic, Cc | Mo $K\alpha$ radiation |
| $a = 31.906 (16) \text{ \AA}$ | $\mu = 0.09 \text{ mm}^{-1}$ |
| $b = 6.130 (3) \text{ \AA}$ | $T = 293 (2) \text{ K}$ |
| $c = 8.726 (4) \text{ \AA}$ | Prism, colorless |
| $\beta = 98.428 (7)^\circ$ | $0.10 \times 0.08 \times 0.05 \text{ mm}$ |
| $V = 1688.3 (15) \text{ \AA}^3$ | |

Data collection

| | |
|---|--|
| Bruker SMART CCD area-detector diffractometer | 1734 independent reflections |
| φ and ω scans | 1100 reflections with $I > 2\sigma(I)$ |
| Absorption correction: none | $R_{\text{int}} = 0.078$ |
| 3808 measured reflections | $\theta_{\text{max}} = 26.5^\circ$ |

Refinement

| | |
|---------------------------------|--|
| Refinement on F^2 | $w = 1/[\sigma^2(F_o^2) + (0.1234P)^2]$ |
| $R[F^2 > 2\sigma(F^2)] = 0.076$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2) = 0.202$ | $(\Delta/\sigma)_{\text{max}} < 0.001$ |
| $S = 0.96$ | $\Delta\rho_{\text{max}} = 0.24 \text{ e \AA}^{-3}$ |
| 1734 reflections | $\Delta\rho_{\text{min}} = -0.27 \text{ e \AA}^{-3}$ |
| 220 parameters | Extinction correction: <i>SHELXL97</i> |
| H-atom parameters constrained | Extinction coefficient: 0.021 (5) |

Table 1

Hydrogen-bond geometry (\AA , $^\circ$).

| $D-H \cdots A$ | $D-H$ | $H \cdots A$ | $D \cdots A$ | $D-H \cdots A$ |
|----------------------|-------|--------------|--------------|----------------|
| $N6-H6A \cdots N4^i$ | 0.86 | 2.19 | 2.968 (7) | 150 |

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

Methyl H atoms were placed in calculated positions, with $C-H = 0.96 \text{ \AA}$ and $U_{\text{iso}}(H) = 1.5U_{\text{eq}}(C)$. Other H atoms were placed in calculated positions, with $C-H = 0.93 \text{ \AA}$ and $N-H = 0.86 \text{ \AA}$, and refined in riding mode, with $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C,N)$. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINTE* (Bruker, 1997); data reduction: *SAINTE*; 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, 1997); software used to prepare material for publication: *SHELXL97*.

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