Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Methyl 2-[2-(5,7-dimethyl-1,2,4-triazolo-[1,5-*a*]pyrimidin-2-ylsulfanylmethyl)phenyl]-3-methoxyacrylate

De-You Teng, Feng-Qin Ji and Wei Huang*

Key Laboratory of Pesticide and Chemical Biology of Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, People's Republic of China

Correspondence e-mail: wuhanhuangwei@163.com

Key indicators

Single-crystal X-ray study
T = 292 K
Mean σ(C–C) = 0.005 Å
R factor = 0.060
wR factor = 0.189
Data-to-parameter ratio = 13.1

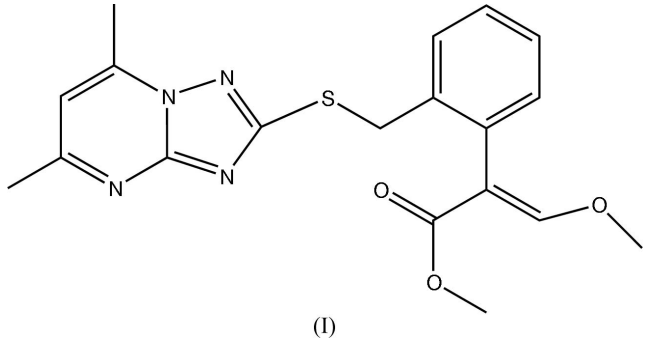
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 11 April 2005
Accepted 25 May 2005
Online 10 June 2005

In the title compound, $C_{19}H_{20}N_4O_3S$, three intramolecular hydrogen bonds and π–π stacking are observed in the crystal structure.

Comment

The strobilurins are an important class of agricultural fungicides, the discovery of which was inspired by a group of natural fungicidal derivatives of *B*-methoxyacrylic acid. Field application of the natural compounds was not possible because of difficulties in their large-scale production and their relative volatility and photochemical instability (Gullino *et al.*, 2000). Therefore, effort was focused on their chemical optimization. Some synthetic analogs are now commercially available, such as azoxystrobin, kresoximmethyl, metominostrobin and trifloxystrobin (Bartlett *et al.*, 2002; Clough, 1993). In order to find novel fungicidal compounds with higher activity, we designed and synthesized the title compound, (I), containing the [1,2,4]triazolo[1,5-*a*]pyrimidine ring. In this paper, we present the X-ray crystallographic analysis of (I).



(I)

As shown in Fig. 1, the heterocycle (N1—C1–C3—N2—N3—C7—N4—C6) is not coplanar with the benzene ring. The angle between their planes is 102.1 (2)°. Two C—H···O and one C—H···N intramolecular hydrogen bonds exist in the crystal structure (Table 1). The angle between the planes of the triazole ring (N2—N3—C7—N4—C6) and the pyrimidine ring (N1—C1—C3—N2—C6) in adjacent molecules is 0.70 (6)°, and the distance between these ring centroids is 3.563 (2) Å (Fig. 2). This suggests the existence of π–π interactions.

Experimental

The title compound was synthesized according to a literature procedure (Clough, 1993). Crystals suitable for single-crystal X-ray diffraction were grown from acetone at 277 K.

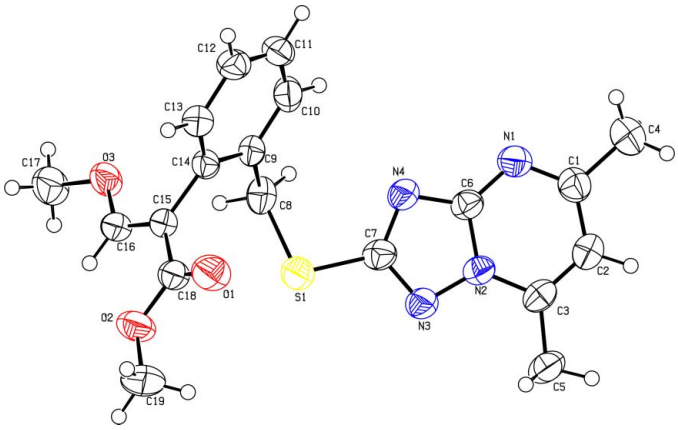


Figure 1
View of the molecule of (I), showing the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented by circles of arbitrary size.

Crystal data

$C_{19}H_{20}N_4O_3S$	$Z = 2$
$M_r = 384.45$	$D_x = 1.356$ Mg m^{-3}
Triclinic, $P\overline{1}$	Mo $K\alpha$ radiation
$a = 8.9163$ (12) Å	Cell parameters from 1142 reflections
$b = 9.5613$ (13) Å	$\theta = 2.3$–$21.1°$
$c = 12.0628$ (17) Å	$\mu = 0.20$ mm^{-1}
$\alpha = 102.881$ (3)°	$T = 292$ (2) K
$\beta = 90.646$ (3)°	Plate, yellow
$\gamma = 109.411$ (3)°	0.30 × 0.20 × 0.04 mm
$V = 941.4$ (2) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	2393 reflections with $I > 2\sigma(I)$
φ and ω scans	$R_{int} = 0.023$
Absorption correction: none	$\theta_{max} = 25.0°$
4766 measured reflections	$h = -10 \rightarrow 7$
3261 independent reflections	$k = -11 \rightarrow 11$
	$l = -14 \rightarrow 14$

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.060$	$w = 1/[\sigma^2(F_o^2) + (0.0954P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.189$	$(\Delta/\sigma)_{max} = 0.031$
$S = 1.11$	$\Delta\rho_{max} = 0.53$ e Å^{-3}
3261 reflections	$\Delta\rho_{min} = -0.63$ e Å^{-3}
248 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
C16—H16···O2	0.93	2.31	2.658 (4)	102
C8—H8B···O3	0.97	2.50	3.242 (4)	133
C8—H8A···N4	0.97	2.54	2.939 (4)	105

All H atoms were initially located in a difference Fourier map. The methyl H atoms were then constrained to an ideal geometry, with C—H distances of 0.96 Å and U_{iso}(H) = 1.5U_{eq}(C), but each group was allowed to rotate freely about its C—C bond. All other H atoms were placed in geometrically idealized positions and constrained to ride on their parent atoms, with C—H distances in the range 0.93–0.97 Å and U_{iso}(H) = 1.2U_{eq}(C).

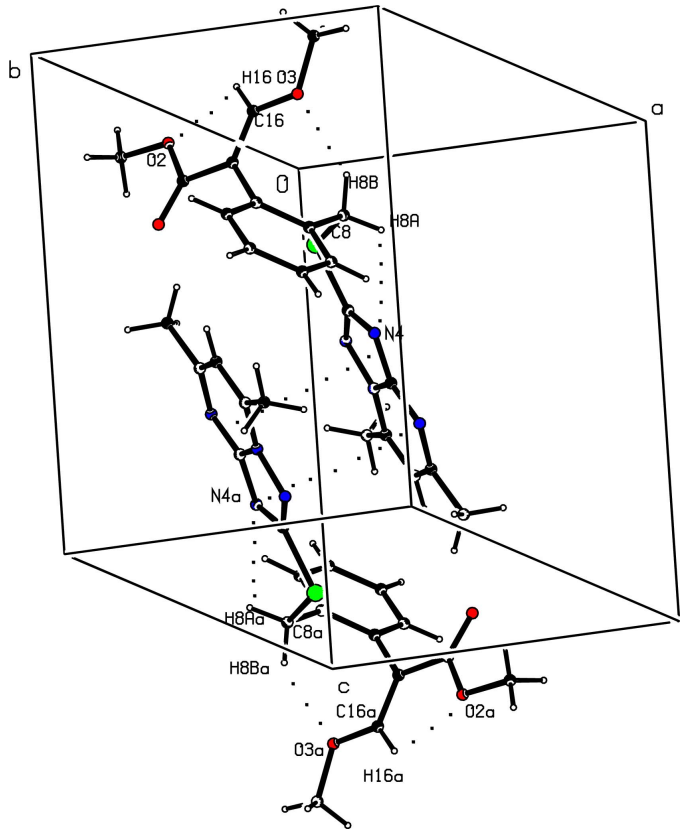


Figure 2
Intramolecular hydrogen bonding and intermolecular π–π stacking between heterocyclic rings, indicated by dotted lines. Atoms labeled with the suffix a are generated by the symmetry operation $(-x, -y, 1 - z)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2001); software used to prepare material for publication: *SHELXTL*.

We are grateful for the kind instruction of Professor Guang-Fu Yang. The authors also acknowledge financial support from the National Key Project for Basic Research (2002CCA00500), the National Natural Science Foundation of China (Nos. 20432010, 20476036 and 20172017), the Program for New Century Excellent Talents in Universities of China and the Program for Excellent Research Groups of Hubei Province (No. 2004ABC002).

References

Bartlett, D. W., Clough, J. M., Godwin, J. R., Hall, A. A., Hamer, M. & Parr-Dobzanski, B. (2002). *Pest Manag. Sci.* **58**, 649–662.
Bruker (1997). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT*. Version 6.01. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2001). *SHELXTL*. Version 6.12. Bruker AXS Inc., Madison, Wisconsin, USA.
Clough, J. M. (1993). *Nat. Prod. Rep.* **10**, 565–574.
Gullino, M. L., Leroux, P. & Smith, C. M. (2000). *Crop Prot.* **19**, 1–11.
Sheldrick, G. M. (1990). *Acta Cryst.* A**46**, 467–473.
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.