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4-Methyl-7-[2-(1*H*-1,2,4-triazol-1-yl)-ethoxy]-2*H*-chromen-2-one

Yi-Yi Zhang, Yuan Shi and Cheng-He Zhou*

Laboratory of Bioorganic and Medicinal Chemistry, School of Chemistry and Chemical Engineering, Southwest University, Chongqing 400715, People's Republic of China
Correspondence e-mail: zhouch@swu.edu.cn

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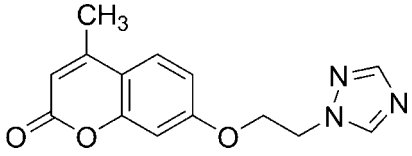
Key indicators: single-crystal X-ray study; T = 173 K; mean σ(C–C) = 0.002 Å; R factor = 0.037; wR factor = 0.097; data-to-parameter ratio = 13.1.

In the title molecule, $C_{14}H_{13}N_3O_3$, the dihedral angle between the triazole ring and coumarin ring system is 73.01 (4)°. The crystal structure is stabilized by weak intermolecular C—H···N and C—H···O hydrogen bonds.

Related literature

For the pharmacological activity of coumarins, see: Wu *et al.* (2009). For details of the synthesis, see: Shi & Zhou (2011).



Experimental

Crystal data

$C_{14}H_{13}N_3O_3$
M_r = 271.27
Monoclinic, $P2_1/n$
a = 11.9861 (17) Å
b = 7.7090 (11) Å
c = 14.132 (2) Å
β = 101.034 (2)°
V = 1281.7 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 173 K
0.40 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer
6501 measured reflections
2390 independent reflections
2134 reflections with $I > 2\sigma(I)$
R_{int} = 0.025

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.097
S = 1.04
2390 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C8—H8···N2^{i}	0.95	2.56	3.453 (2)	157
C9—H9···N3^{ii}	0.95	2.49	3.380 (2)	157
C13—H13···O1^{iii}	0.95	2.48	3.408 (2)	165
C13—H13···O2^{iii}	0.95	2.59	3.410 (2)	144
C14—H14···O3^{iv}	0.95	2.55	3.481 (2)	166

Symmetry codes: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x+\frac{1}{2}, -y+\frac{5}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$; (iv) $x, y+1, z$.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: LH5217).

References

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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Wu, L., Wang, X., Xu, W., Farzaneh, F. & Xu, R. (2009). *Curr. Med. Chem.* **16**, 4236–4260.

supporting information

Acta Cryst. (2011). E**67**, o892 [doi:10.1107/S1600536811009159]

4-Methyl-7-[2-(1*H*-1,2,4-triazol-1-yl)ethoxy]-2*H*-chromen-2-one

Yi-Yi Zhang, Yuan Shi and Cheng-He Zhou

S1. Comment

Coumarins and their derivatives have attracted considerable attention due to their extensively biological activities such as antibacterial, antifungal, antiviral, anti-tubercular, anti-malarial, anticoagulant, anti-inflammatory, anticancer and antioxidant properties (Wu, *et al.*, 2009; Shi, *et al.*, 2011). In view of the therapeutic potentials of coumarins, we synthesized the title compound (I). Herein we report its crystal structure.

The molecular structure of the title compound is shown in Fig. 1. The dihedral angle between the triazole ring and coumarin ring system is 73.01 (4)°. The crystal structure is stabilized by weak intermolecular C—H···N and C—H···O hydrogen bonds.

S2. Experimental

Compound (I) was synthesized according to the procedure of Shi & Zhou (2011). Single crystals were grown by slow evaporation of a solution of (I) in $CDCl_3$ at room temperature.

S3. Refinement

Hydrogen atoms were placed in idealized positions and treated as riding, with C—H = 0.95 Å (CH), 0.99 Å (CH_2) U_{iso}(H) = 1.2 U_{eq}(CH, CH_2) and 0.98 Å (CH_3), U_{iso}(H) = 1.5U_{eq}(CH_3).

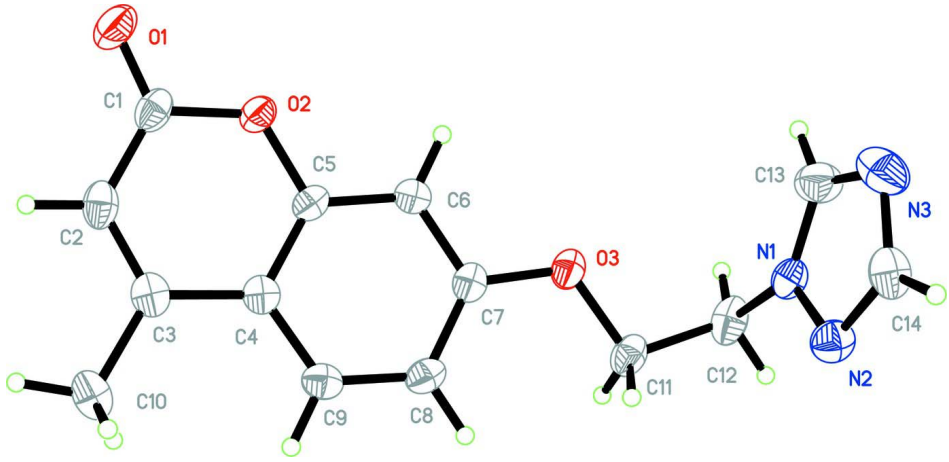

Figure 1

The molecular structure of (I) with displacement ellipsoids are drawn at the 50% probability level.

4-Methyl-7-[2-(1*H*-1,2,4-triazol-1-yl)ethoxy]-2*H*-chromen-2-one

Crystal data

$C_{14}H_{13}N_3O_3$
$M_r = 271.27$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 11.9861\ (17)$ Å
$b = 7.7090\ (11)$ Å
$c = 14.132\ (2)$ Å
$\beta = 101.034\ (2)°$
$V = 1281.7\ (3)$ Å^3
$Z = 4$
$F(000) = 568$
$D_x = 1.406$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3660 reflections
$\theta = 2.5–28.1°$
$\mu = 0.10$ mm^{-1}
$T = 173$ K
Block, colourless
0.40 × 0.30 × 0.24 mm

Data collection

Bruker SMART CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
6501 measured reflections
2390 independent reflections
2134 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.0°$
$h = -14\rightarrow14$
$k = -9\rightarrow9$
$l = -17\rightarrow14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.037$
$wR(F^2) = 0.097$
$S = 1.04$
2390 reflections
182 parameters
0 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0489P)^2 + 0.3468P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.23$ e Å^{-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 based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ 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	0.34092 (11)	0.63715 (16)	1.03382 (10)	0.0285 (3)
C2	0.44570 (12)	0.61742 (16)	1.10231 (10)	0.0291 (3)
H2	0.4448	0.5553	1.1602	0.035*
C3	0.54494 (11)	0.68343 (16)	1.08755 (9)	0.0261 (3)
C4	0.54683 (10)	0.77458 (15)	0.99847 (9)	0.0228 (3)

C5	0.44581 (10)	0.78927 (15)	0.93081 (9)	0.0222 (3)
C6	0.43918 (10)	0.87313 (15)	0.84385 (9)	0.0233 (3)
H6	0.3692	0.8796	0.7992	0.028*
C7	0.53705 (11)	0.94803 (15)	0.82283 (9)	0.0232 (3)
C8	0.64008 (10)	0.93534 (16)	0.88806 (10)	0.0258 (3)
H8	0.7071	0.9852	0.8732	0.031*
C9	0.64365 (11)	0.84983 (16)	0.97420 (10)	0.0258 (3)
H9	0.7140	0.8418	1.0184	0.031*
C10	0.65229 (12)	0.66473 (19)	1.16165 (10)	0.0351 (3)
H10A	0.6375	0.5922	1.2149	0.053*
H10B	0.6783	0.7795	1.1864	0.053*
H10C	0.7111	0.6103	1.1320	0.053*
C11	0.62329 (11)	1.10015 (17)	0.70725 (10)	0.0296 (3)
H11A	0.6776	1.0054	0.7024	0.036*
H11B	0.6612	1.1859	0.7549	0.036*
C12	0.58548 (13)	1.18489 (17)	0.61091 (10)	0.0326 (3)
H12A	0.6525	1.2038	0.5807	0.039*
H12B	0.5330	1.1058	0.5687	0.039*
C13	0.42086 (12)	1.3931 (2)	0.58744 (11)	0.0379 (4)
H13	0.3631	1.3152	0.5581	0.046*
C14	0.50929 (12)	1.61203 (18)	0.64494 (10)	0.0328 (3)
H14	0.5252	1.7284	0.6651	0.039*
N1	0.52866 (9)	1.35020 (14)	0.61733 (8)	0.0256 (3)
N2	0.58838 (9)	1.49167 (14)	0.65533 (8)	0.0308 (3)
N3	0.40436 (11)	1.55923 (18)	0.60384 (10)	0.0440 (3)
O1	0.24796 (9)	0.58794 (14)	1.04329 (8)	0.0415 (3)
O2	0.34566 (7)	0.71985 (11)	0.94832 (6)	0.0267 (2)
O3	0.52351 (8)	1.03232 (12)	0.73646 (6)	0.0278 (2)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0340 (7)	0.0207 (6)	0.0344 (8)	−0.0007 (5)	0.0152 (6)	0.0017 (5)
C2	0.0418 (8)	0.0215 (6)	0.0263 (7)	0.0029 (5)	0.0123 (6)	0.0015 (5)
C3	0.0347 (7)	0.0188 (6)	0.0253 (7)	0.0038 (5)	0.0067 (5)	−0.0041 (5)
C4	0.0271 (6)	0.0177 (6)	0.0240 (6)	0.0019 (5)	0.0060 (5)	−0.0036 (5)
C5	0.0232 (6)	0.0173 (6)	0.0281 (7)	−0.0012 (5)	0.0097 (5)	−0.0029 (5)
C6	0.0228 (6)	0.0220 (6)	0.0247 (7)	0.0005 (5)	0.0035 (5)	−0.0021 (5)
C7	0.0290 (6)	0.0181 (6)	0.0243 (7)	0.0014 (5)	0.0094 (5)	−0.0020 (5)
C8	0.0227 (6)	0.0231 (6)	0.0335 (7)	−0.0014 (5)	0.0100 (5)	−0.0023 (5)
C9	0.0233 (6)	0.0229 (6)	0.0302 (7)	0.0017 (5)	0.0031 (5)	−0.0035 (5)
C10	0.0429 (8)	0.0334 (8)	0.0268 (7)	0.0034 (6)	0.0009 (6)	0.0019 (6)
C11	0.0320 (7)	0.0241 (6)	0.0371 (8)	0.0015 (5)	0.0175 (6)	0.0023 (6)
C12	0.0465 (8)	0.0242 (7)	0.0321 (8)	0.0010 (6)	0.0205 (6)	−0.0015 (6)
C13	0.0297 (7)	0.0448 (9)	0.0377 (8)	−0.0036 (6)	0.0025 (6)	−0.0003 (7)
C14	0.0435 (8)	0.0268 (7)	0.0289 (7)	0.0043 (6)	0.0090 (6)	−0.0007 (6)
N1	0.0294 (6)	0.0252 (5)	0.0238 (6)	−0.0027 (4)	0.0093 (4)	−0.0006 (4)
N2	0.0309 (6)	0.0274 (6)	0.0341 (6)	−0.0019 (5)	0.0061 (5)	−0.0039 (5)

N3	0.0365 (7)	0.0479 (8)	0.0460 (8)	0.0129 (6)	0.0040 (6)	0.0032 (6)
O1	0.0359 (6)	0.0416 (6)	0.0514 (7)	−0.0049 (5)	0.0192 (5)	0.0119 (5)
O2	0.0243 (5)	0.0264 (5)	0.0305 (5)	−0.0035 (4)	0.0083 (4)	0.0031 (4)
O3	0.0305 (5)	0.0279 (5)	0.0266 (5)	−0.0017 (4)	0.0094 (4)	0.0039 (4)

Geometric parameters (Å, º)

C1—O1	1.2085 (16)	C10—H10A	0.9800
C1—O2	1.3769 (16)	C10—H10B	0.9800
C1—C2	1.439 (2)	C10—H10C	0.9800
C2—C3	1.3463 (19)	C11—O3	1.4364 (15)
C2—H2	0.9500	C11—C12	1.500 (2)
C3—C4	1.4457 (18)	C11—H11A	0.9900
C3—C10	1.5023 (19)	C11—H11B	0.9900
C4—C5	1.3964 (18)	C12—N1	1.4560 (17)
C4—C9	1.3975 (17)	C12—H12A	0.9900
C5—C6	1.3774 (18)	C12—H12B	0.9900
C5—O2	1.3793 (14)	C13—N1	1.3223 (18)
C6—C7	1.3896 (17)	C13—N3	1.323 (2)
C6—H6	0.9500	C13—H13	0.9500
C7—O3	1.3647 (15)	C14—N2	1.3145 (17)
C7—C8	1.3960 (18)	C14—N3	1.344 (2)
C8—C9	1.3778 (19)	C14—H14	0.9500
C8—H8	0.9500	N1—N2	1.3576 (15)
C9—H9	0.9500		
O1—C1—O2	115.86 (12)	H10A—C10—H10B	109.5
O1—C1—C2	126.63 (13)	C3—C10—H10C	109.5
O2—C1—C2	117.50 (11)	H10A—C10—H10C	109.5
C3—C2—C1	122.62 (12)	H10B—C10—H10C	109.5
C3—C2—H2	118.7	O3—C11—C12	107.20 (11)
C1—C2—H2	118.7	O3—C11—H11A	110.3
C2—C3—C4	118.69 (12)	C12—C11—H11A	110.3
C2—C3—C10	121.34 (13)	O3—C11—H11B	110.3
C4—C3—C10	119.97 (12)	C12—C11—H11B	110.3
C5—C4—C9	116.76 (12)	H11A—C11—H11B	108.5
C5—C4—C3	118.66 (11)	N1—C12—C11	112.86 (11)
C9—C4—C3	124.58 (12)	N1—C12—H12A	109.0
C6—C5—O2	116.01 (11)	C11—C12—H12A	109.0
C6—C5—C4	122.92 (11)	N1—C12—H12B	109.0
O2—C5—C4	121.07 (11)	C11—C12—H12B	109.0
C5—C6—C7	118.60 (11)	H12A—C12—H12B	107.8
C5—C6—H6	120.7	N1—C13—N3	110.86 (13)
C7—C6—H6	120.7	N1—C13—H13	124.6
O3—C7—C6	115.36 (11)	N3—C13—H13	124.6
O3—C7—C8	124.24 (11)	N2—C14—N3	115.46 (13)
C6—C7—C8	120.40 (12)	N2—C14—H14	122.3
C9—C8—C7	119.40 (11)	N3—C14—H14	122.3

C9—C8—H8	120.3	C13—N1—N2	109.53 (11)
C7—C8—H8	120.3	C13—N1—C12	129.74 (12)
C8—C9—C4	121.91 (12)	N2—N1—C12	120.68 (11)
C8—C9—H9	119.0	C14—N2—N1	102.03 (11)
C4—C9—H9	119.0	C13—N3—C14	102.12 (12)
C3—C10—H10A	109.5	C1—O2—C5	121.37 (10)
C3—C10—H10B	109.5	C7—O3—C11	117.86 (10)

O1—C1—C2—C3	−176.91 (13)	C5—C4—C9—C8	0.34 (18)
O2—C1—C2—C3	3.28 (19)	C3—C4—C9—C8	−179.93 (11)
C1—C2—C3—C4	−1.36 (19)	O3—C11—C12—N1	74.23 (14)
C1—C2—C3—C10	178.33 (12)	N3—C13—N1—N2	−0.17 (17)
C2—C3—C4—C5	−0.56 (17)	N3—C13—N1—C12	−177.64 (13)
C10—C3—C4—C5	179.75 (11)	C11—C12—N1—C13	−111.33 (16)
C2—C3—C4—C9	179.72 (12)	C11—C12—N1—N2	71.44 (15)
C10—C3—C4—C9	0.02 (18)	N3—C14—N2—N1	0.17 (16)
C9—C4—C5—C6	−0.06 (18)	C13—N1—N2—C14	0.00 (15)
C3—C4—C5—C6	−179.80 (11)	C12—N1—N2—C14	177.75 (11)
C9—C4—C5—O2	−179.74 (10)	N1—C13—N3—C14	0.25 (16)
C3—C4—C5—O2	0.51 (17)	N2—C14—N3—C13	−0.26 (17)
O2—C5—C6—C7	179.02 (10)	O1—C1—O2—C5	176.87 (11)
C4—C5—C6—C7	−0.68 (18)	C2—C1—O2—C5	−3.29 (17)
C5—C6—C7—O3	−178.52 (10)	C6—C5—O2—C1	−178.20 (11)
C5—C6—C7—C8	1.15 (18)	C4—C5—O2—C1	1.50 (17)
O3—C7—C8—C9	178.75 (11)	C6—C7—O3—C11	−175.04 (10)
C6—C7—C8—C9	−0.89 (18)	C8—C7—O3—C11	5.30 (17)
C7—C8—C9—C4	0.13 (19)	C12—C11—O3—C7	179.81 (10)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C8—H8···N2^{i}	0.95	2.56	3.453 (2)	157
C9—H9···N3^{ii}	0.95	2.49	3.380 (2)	157
C13—H13···O1^{iii}	0.95	2.48	3.408 (2)	165
C13—H13···O2^{iii}	0.95	2.59	3.410 (2)	144
C14—H14···O3^{iv}	0.95	2.55	3.481 (2)	166

Symmetry codes: (i) −*x*+3/2, *y*−1/2, −*z*+3/2; (ii) *x*+1/2, −*y*+5/2, *z*+1/2; (iii) −*x*+1/2, *y*+1/2, −*z*+3/2; (iv) *x*, *y*+1, *z*.