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4-[3-(1,2,4-Triazol-1-yl)propionyl]phenyl 4-fluorobenzoate

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In the title compound, $C_{18}H_{14}FN_3O_3$, the dihedral angles made by the triazole ring with the plane of the central benzene ring and the *p*-fluorophenylcarbonyl group are 82.09 (2) and 82.05 (2)°, respectively. There are weak C—H···O intra- and intermolecular interactions in the crystal structure, which contribute to the stability.

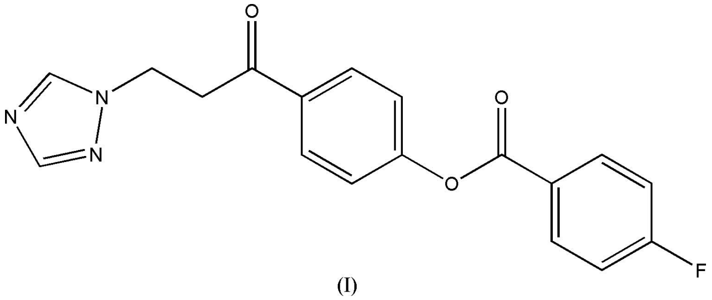
Key indicators

Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.036
wR factor = 0.093
Data-to-parameter ratio = 8.6

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

Comment

Triazole rings appear frequently in the structures of various natural products and biologically active compounds, notably thiamine (vitamin B), penicillins and antibiotics, such as micrococcin (James & Watson, 1966). Triazole derivatives have also attracted considerable attention in industry and agriculture because of their significant biological activities (Zhang *et al.*, 2002). In this paper, we report the structure of the title compound, (I).



(I)

In the molecule of (I) (Fig. 1), the bond lengths and angles are generally normal in the benzene and triazole rings (Ji *et al.*, 2002). The C1—O1 and C14—O3 bond lengths of 1.200 (3) and 1.216 (3) Å, respectively (Table 1), are close to the typical C=O double-bond length. Atom C16 lies in the plane of the triazole ring, and atoms O3, C11, C14 and C15 are coplanar (plane *P*1). The dihedral angles formed by the triazole and C8–C13 rings with *P*1 are 81.20 (3) and 5.16 (2)°, respectively. Atom C1 lies in the plane of the C2–C7 benzene ring, and atoms O1, O2, C1, C2 and C8 are coplanar (plane *P*2). The dihedral angles formed by the triazole and C2–C7 rings with *P*2 are 78.75 (3) and 82.05 (2)°, respectively.

The structure of (I) shows a number of weak C—H···O intra- and intermolecular interactions (Table 2) which stabilize the crystal structure.

Experimental

1-(4-Hydroxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one was prepared according to the method reported by Ogata *et al.* (1987). The title compound was prepared by the reaction of 1-(4-hydroxyphenyl)-3-(1*H*-1,2,4-triazol-1-yl)propan-1-one (2.17 g, 10 mmol) with 4-fluorobenzoyl chloride (1.59 g, 10 mmol) in acetone. Single crystals of (I) suitable for X-ray measurements were obtained by recrystallization from chloroform–ethyl acetate (1:3, *v*/*v*) at room temperature (m.p. 437–438 K). ^{1}H NMR (600 MHz, acetone-d^6, δ, p.p.m.): 7.12–8.15 (10H, *m*, Ar), 3.03–3.92 (4H, *m*, N—CH2—CH2—O). Analysis, calculated for $C_{18}H_{14}FN_3O_3$: C 63.71, H 4.16, N 12.38%; found: C 63.67, H 4.22, N 12.71%.

Crystal data

$C_{18}H_{14}FN_3O_3$
M_r = 339.32
Orthorhombic, $P2_12_12_1$
a = 5.8352 (11) Å
b = 8.0741 (14) Å
c = 34.311 (7) Å
V = 1616.5 (5) Å^3
Z = 4
D_x = 1.394 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2217 reflections
θ = 3.1–21.3°
μ = 0.11 mm^{-1}
T = 294 (2) K
Block, colourless
0.38 × 0.20 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min}$ = 0.975, $T_{\max}$ = 0.987
9128 measured reflections
1953 independent reflections
1254 reflections with $I > 2\sigma(I)$
$R_{\rm int}$ = 0.040
$\theta_{\max}$ = 26.3°
$h = -7 \rightarrow 5$
$k = -8 \rightarrow 10$
$l = -35 \rightarrow 42$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
S = 1.02
1953 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0379P)^2 + 0.2678P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max}$ = 0.001
$\Delta\rho_{\max}$ = 0.14 e Å^{-3}
$\Delta\rho_{\min}$ = −0.17 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

F1—C5	1.357 (3)	O2—C8	1.407 (3)
N1—C16	1.458 (4)	O3—C14	1.216 (3)
O1—C1	1.200 (3)	C14—C15	1.500 (4)
O2—C1	1.358 (3)	C15—C16	1.515 (4)
C18—N1—C16	130.7 (3)	C13—C8—O2	118.9 (3)
N2—N1—C16	120.0 (2)	C9—C8—O2	119.4 (3)
C1—O2—C8	117.7 (2)	O3—C14—C11	120.2 (3)
O1—C1—O2	122.5 (3)	O3—C14—C15	120.9 (3)
O1—C1—C2	126.0 (3)	C11—C14—C15	118.8 (3)
O2—C1—C2	111.4 (3)	C14—C15—C16	114.6 (3)
F1—C5—C6	118.4 (3)	N1—C16—C15	111.2 (3)
F1—C5—C4	118.0 (3)		
C10—C11—C14—O3	−6.8 (4)	C18—N1—C16—C15	−104.6 (4)
O3—C14—C15—C16	7.4 (4)	N2—N1—C16—C15	72.4 (3)

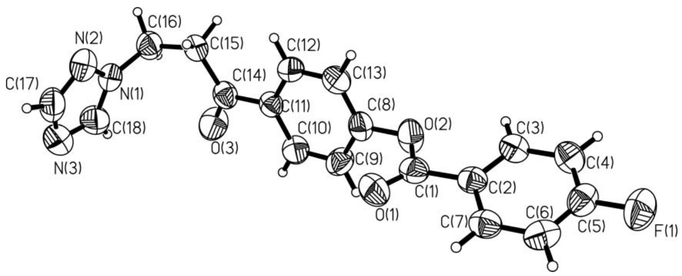


Figure 1
The structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. H atoms are drawn as small spheres of arbitrary radii.

Table 2
Hydrogen-bond geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
C3—H3$\cdots$O2	0.93	2.42	2.731 (3)	100
C13—H13$\cdots$O1$^{\rm i}$	0.93	2.43	3.180 (4)	137

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

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.97 Å, and included in the final cycles of refinement using a riding model, with $U_{\rm iso}$(H) = 1.2$U_{\rm eq}$(C). In the absence of significant anomalous dispersion effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); 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, 1999); software used to prepare material for publication: *SHELXTL*.

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