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N′-(2-Fluorobenzylidene)-2-(quinolin-8-yloxy)-acetohydrazide methanol solvate

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Key indicators

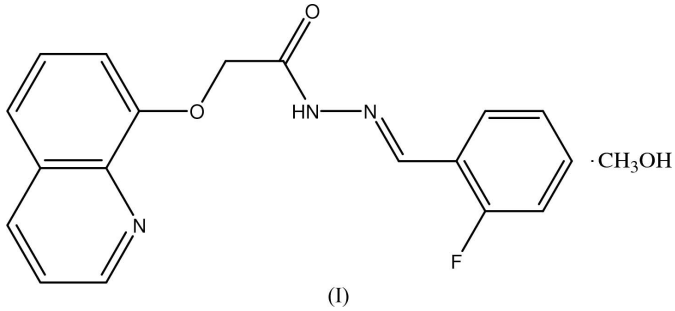
Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.042
wR factor = 0.122
Data-to-parameter ratio = 13.7

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

In the title compound, $C_{18}H_{14}FN_3O_2\cdot CH_4O$, all bond lengths and angles are within normal ranges. The $C_{18}H_{14}FN_3O_2$ molecule is essentially planar, with a dihedral angle of 7.83 (7)° between the planes of the benzene ring and the quinoline group. Each methanol molecule is linked to one $C_{18}H_{14}FN_3O_2$ molecule *via* intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds.

Comment

As part of our ongoing search for good extractants of metal ions or a biologically active material, the title compound, (I), was obtained in the reaction of quinolin-8-yloxyacetic acid hydrazide and 2-fluorobenzaldehyde. We report here the crystal structure of (I).



(I)

The bond lengths and angles in (I) (Table 1) are within normal ranges (Allen *et al.*, 1987), and are comparable to those in the related compound *N*,*N*-diphenyl-2-(quinolin-8-yloxy)acetamide monohydrate (Wen *et al.*, 2005). The $C_{18}H_{14}FN_3O_2$ molecule is essentially planar, with a dihedral angle of 7.83 (7)° between the planes of the benzene ring and the quinoline group. The intramolecular N2—H2*A*···O1 hydrogen bond, forming a five-membered ring, contributes to the planarity of the title molecule. Each methanol molecule is linked to one $C_{18}H_{14}FN_3O_2$ molecule *via* intermolecular N—H···O, O—H···O and O—H···N hydrogen bonds (Table 2 and Fig. 2).

Experimental

Quinolin-8-yloxyacetic acid hydrazide (2.18 g, 10 mmol), 2-fluorobenzaldehyde (1.30 g, 10.5 mmol), ethanol (40 ml) and some drops of acetic acid were added to a 100 ml flask, and refluxed for 3 h. After cooling to room temperature, the mixture was filtered. Colourless single crystals suitable for X-ray diffraction study were obtained by slow evaporation of a tetrahydrofuran–methanol (1:2, *v*/*v*) solution over a period of 5 d.

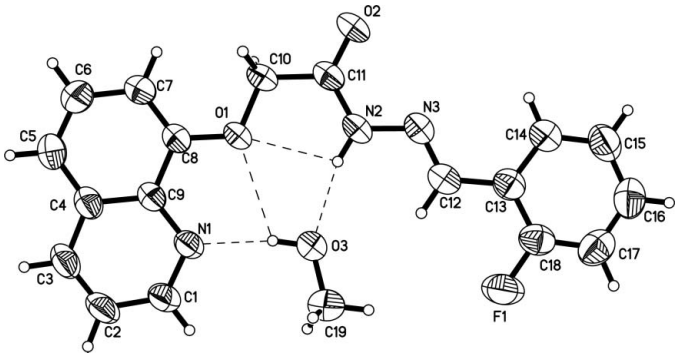


Figure 1
View of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The dashed lines indicate hydrogen bonds.

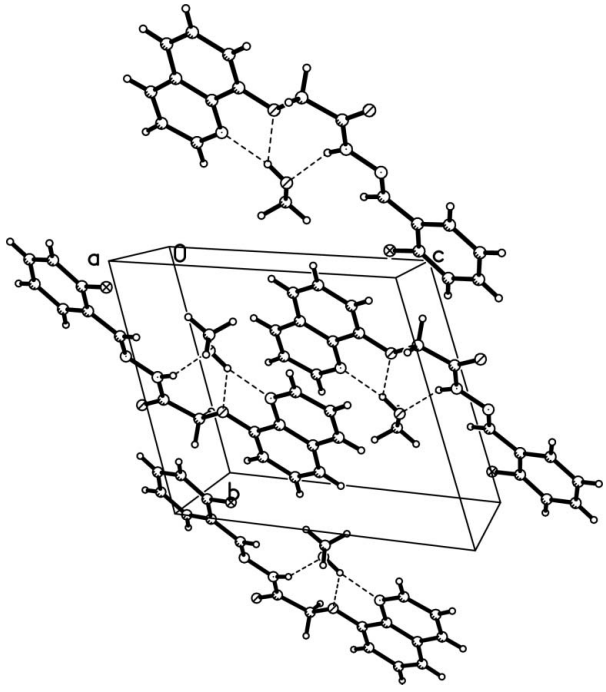


Figure 2
Packing diagram of the title compound, showing intermolecular hydrogen bonds (dashed lines).

Crystal data

$C_{18}H_{14}FN_3O_2{\cdot}CH_4O$
M_r = 355.36
Triclinic, $P\overline{1}$
a = 9.071 (2) Å
b = 9.546 (2) Å
c = 11.506 (3) Å
α = 66.450 (4)°
β = 71.709 (4)°
γ = 74.490 (4)°
V = 855.6 (3) Å^3
Z = 2
D_x = 1.379 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2286 reflections
θ = 2.4–26.0°
μ = 0.10 mm^{-1}
T = 293 (2) K
Column, colourless
0.42 × 0.27 × 0.13 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.958, T_{max} = 0.987
4778 measured reflections
3286 independent reflections
2742 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
θ_{max} = 26.1°
$h = -11 \rightarrow 11$
$k = -6 \rightarrow 11$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.122
S = 1.06
3286 reflections
239 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.0967P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

F1—C18	1.3588 (18)	N2—C11	1.3451 (19)
O1—C8	1.3723 (16)	N2—N3	1.3819 (17)
O1—C10	1.4241 (16)	N3—C12	1.271 (2)
O2—C11	1.2167 (16)		
C8—O1—C10	115.37 (11)	C12—N3—N2	115.58 (12)
C11—N2—N3	118.17 (11)	O1—C10—C11	113.46 (12)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	2.33	2.698 (2)	106
N2—H2A···O3	0.86	2.06	2.879 (2)	158
O3—H1O3···O1	0.90 (3)	2.50 (3)	3.011 (2)	116 (2)
O3—H1O3···N1	0.90 (3)	1.88 (3)	2.771 (2)	169 (2)

The solvent H atoms were located in a difference Fourier map, while the other H atoms were positioned geometrically. The hydroxy atom H1O3 was refined freely. All other H atoms were allowed to ride on their parent atoms, with C—H = 0.93–0.97 Å, N—H = 0.86 Å and U_{iso}(H) = 1.2–1.5U_{eq}(parent atom).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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