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N-(4-Ethoxyphenyl)-2-(quinolin-8-yloxy)acetamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.002 Å
R factor = 0.043
wR factor = 0.115
Data-to-parameter ratio = 14.8

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

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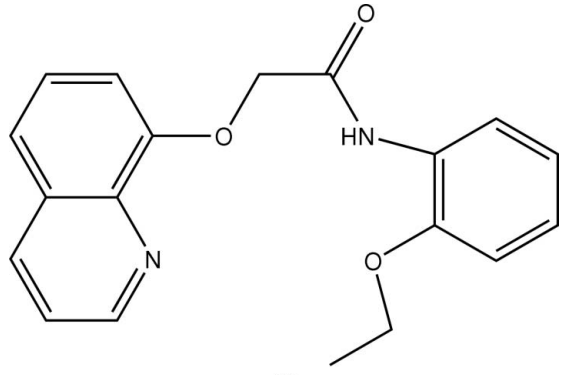
The molecule of the title compound, $C_{19}H_{18}N_2O_3$, shows a nearly planar conformation, with a dihedral angle of 8.46 (6)° between the benzene ring and the quinoline moiety. The molecules are linked into dimers by C—H···O interactions.

Comment

As part of our studies on amide compounds, the title compound, (I), was synthesized and the structure was determined. The bond lengths (Table 1) are comparable with those in the related compound, *N*-(4-methoxyphenyl)-2-(quinolin-8-yloxy)acetamide monohydrate, (II) (Wen *et al.*, 2005). The non-H atoms in (I) show a nearly planar conformation, with a dihedral angle of 8.46 (6)° between the benzene ring and the quinoline moiety, while the corresponding value in (II) is 67.06 (7)°. There are three intramolecular hydrogen bonds (Table 2), forming two five-membered and one six-membered rings (Fig. 1), which contribute to the planarity of the whole molecule. In the crystal structure, the molecules are linked into a dimer by a further C—H···O hydrogen bond (Table 2 and Fig. 2).



(I)

Experimental

The title compound was prepared according to the literature method of Wen *et al.* (2005). Colorless single crystals suitable for X-ray diffraction were obtained by slow evaporation of a petroleum ether–ethyl acetate (1:3, *v*/*v*) solution over 5 d.

Crystal data

$C_{19}H_{18}N_2O_3$
M_r = 322.35
Monoclinic, $P2_1/c$
a = 8.0480 (13) Å
b = 8.5248 (14) Å
c = 23.821 (4) Å
β = 91.676 (2)°
V = 1633.6 (5) Å^3
Z = 4
D_x = 1.311 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4032 reflections
θ = 2.5–25.7°
μ = 0.09 mm^{-1}
T = 293 (2) K
Plate, colourless
0.53 × 0.27 × 0.17 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.954, T_{max} = 0.985
8662 measured reflections
3220 independent reflections
2658 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 26.1°
$h = -9 \rightarrow 9$
$k = -7 \rightarrow 10$
$l = -29 \rightarrow 28$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.115
S = 1.03
3220 reflections
217 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0629P)^2 + 0.1712P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

Table 1
Selected bond lengths (Å).

O1—C8	1.3631 (15)	N2—C11	1.3422 (16)
O1—C10	1.4176 (15)	N2—C12	1.4101 (15)
O2—C11	1.2142 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···O1	0.86	2.17	2.623 (1)	112
N2—H2A···O3	0.86	2.19	2.602 (1)	109
C13—H13A···O2	0.93	2.31	2.903 (2)	121
C14—H14A···O2^{i}	0.93	2.54	3.300 (2)	139

Symmetry code: (i) $-x-1, -y+2, -z$.

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C or N) [U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms].

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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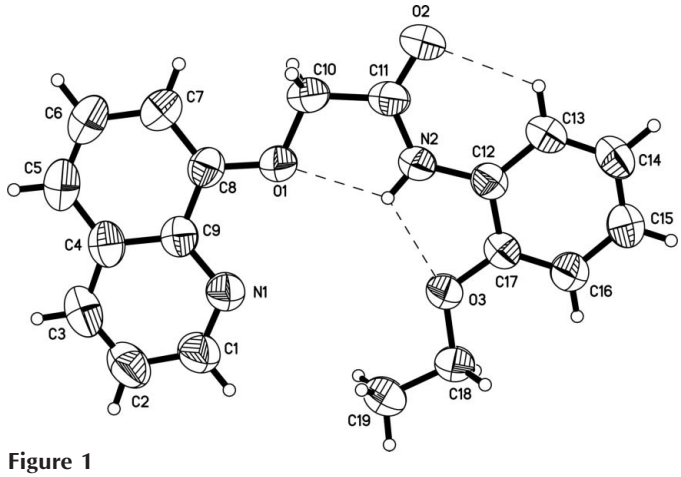

Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme. The dashed lines indicate hydrogen bonds.

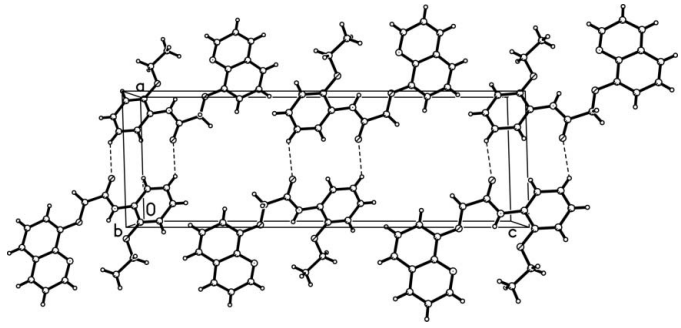

Figure 2
A view down the *b* axis, showing the hydrogen-bonded dimers. Hydrogen bonds are indicated by dashed lines.

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