Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-(4-Ethoxyphenylamino)-2-oxo-1,2-dihydroquinoline

Victor B. Rybakov,[a]* Vladimir V. Chernyshev,[a] Igor V. Ukrainets,[b] Peter A. Bezugly,[b] Lyudmila V. Sidorenko[b] and Nicola Skaif[b]

[a]Department of Chemistry, Moscow State University, 119899 Moscow, Russian Federation, and [b]Pharmaceutical Chemistry Department, Ukrainian National Academy of Pharmacy, 61002 Kharkov, Ukraine

Correspondence e-mail: rybakov@biocryst.phys.msu.su

Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.046
wR factor = 0.104
Data-to-parameter ratio = 10.8

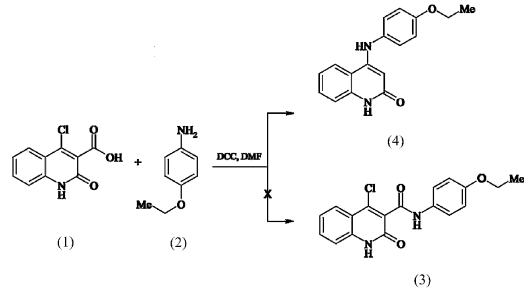
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 8 May 2001
Accepted 2 July 2001
Online 13 July 2001

The reaction product of 4-chloro-2-oxo-1,2-dihydroquinoline-3-carboxylic acid with *p*-phenetidine is 4-(4-ethoxyphenylamino)-2-oxo-1,2-dihydroquinoline, $C_{17}H_{16}N_2O_2$. The molecules form centrosymmetric hydrogen-bonded dimers.

Comment

N,*N*′-dicyclohexylcarbodiimide (DCC) (Kurzer & Douraghi-Zaden, 1967) is widely used in organic chemistry for the synthesis of amides of carboxylic acids. We investigated the possibility of using this condensing reagent for the synthesis of 4-chloro-2-oxo-1,2-dihydroquinoline-3-carboxamide (3) (see scheme below), which was supposed to possess bioactive properties. We carried out the reaction between 4-chloro-2-oxo-1,2-dihydroquinoline (1) with *p*-phenetidine (2) in a boiling mixture of *N*,*N*-dimethylformamide (DMF) and DCC, and obtained 4-(4-ethoxyphenylamino)-2-oxo-1,2-dihydroquinoline, $C_{17}H_{16}N_2O_2$ (4) instead of (3).



The X-ray single-crystal analysis showed that the 10-membered heterobicycle (N1–C10) (Fig. 1) is planar to within 0.06 Å, the O21 and N41 atoms showing small displacements from its least-squares plane [0.135 (2) and −0.166 (3) Å respectively]. The C11 atom also lies essentially in the same plane, as indicated by the C5—C4—N41—C11 torsion angle of −177.1 (2)°. The C11–C16 phenyl ring, however, is rotated out of the dihydroquinoline plane and forms a dihedral angle of 63.63 (4)° with the latter.

The N1—H1···O21 hydrogen bond [H1···O21^{i} 1.86 (2), N1···O21^{i} 2.784 (2) Å and N1—H1···O21^{i} 168 (2)°; symmetry operation (i) $1-x$, $1-y$, $1-z$] links the molecules in the crystal into centrosymmetric dimers.

Experimental

2.23 g (0.01 mol) of (1) was refluxed for 2 h in 30 ml of *N*,*N*-dimethylformamide (DMF) with 1.51 g (0.011 mol) of *p*-phenetidine and 2.26 g (0.011 mol) of DCC. 4-(4-ethoxyphenylamino)-2-oxo-1,2-dihydroquinoline, $C_{17}H_{16}N_2O_2$ (4) was obtained (2.07 g, yield 74%) and was recrystallized from DMF.

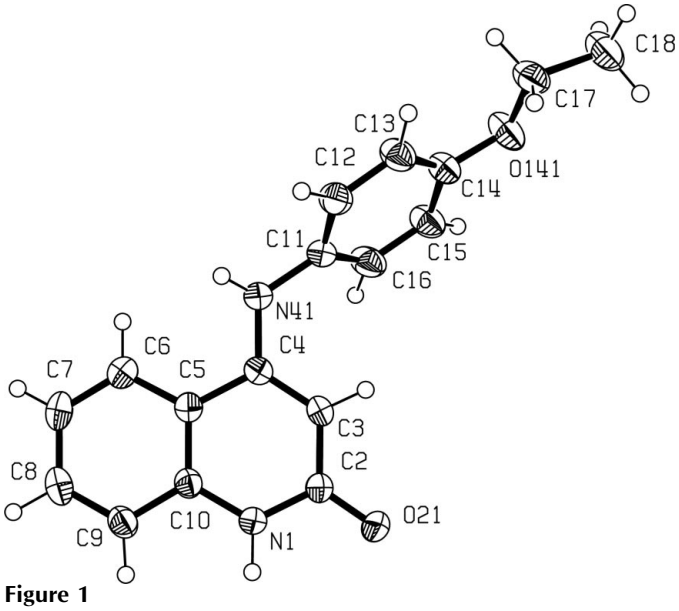


Figure 1
ORTEP-3 (Farrugia, 1998*b*) plot of the molecule of the title compound. Displacement ellipsoids are drawn at the 50% probability level

Crystal data

$C_{17}H_{16}N_2O_2$
M_r = 280.32
Triclinic, $P\overline{1}$
a = 7.075 (3) Å
b = 8.783 (5) Å
c = 12.469 (5) Å
α = 105.85 (4)°
β = 93.44 (3)°
γ = 106.89 (3)°
V = 705.0 (6) Å^3
Z = 2
D_x = 1.321 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 22 reflections
θ = 15.7–17.7°
μ = 0.09 mm^{-1}
T = 293 (2) K
Prism, colourless
0.43 × 0.33 × 0.18 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
ω scans
Absorption correction: none
2956 measured reflections
2765 independent reflections
1912 reflections with $I > 2\sigma(I)$
R_{int} = 0.017
θ_{max} = 26.0°
$h = -8 \rightarrow 8$
$k = 0 \rightarrow 10$
$l = -15 \rightarrow 14$
2 standard reflections
every 200 reflections
frequency: 125 min
intensity decay: 1%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.104
S = 1.10
2765 reflections
255 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.05P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.049
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Extinction correction: *SHELXL*97 (Sheldrick, 1997)
Extinction coefficient: 0.029 (5)

Table 1
Selected geometric parameters (Å, °).

N1—C2	1.363 (2)	C8—C9	1.362 (3)
N1—C10	1.375 (2)	C9—C10	1.402 (2)
C2—O21	1.254 (2)	C11—C12	1.375 (3)
C2—C3	1.419 (2)	C11—C16	1.392 (3)
C3—C4	1.359 (2)	C12—C13	1.386 (3)
C4—N41	1.378 (2)	C13—C14	1.382 (3)
C4—C5	1.455 (2)	C14—O141	1.367 (2)
N41—C11	1.419 (2)	C14—C15	1.391 (3)
C5—C6	1.396 (3)	O141—C17	1.428 (2)
C5—C10	1.400 (2)	C15—C16	1.368 (3)
C6—C7	1.373 (3)	C17—C18	1.497 (3)
C7—C8	1.391 (3)		
C2—N1—C10	123.42 (15)	N1—C10—C5	120.22 (15)
O21—C2—N1	119.2 (2)	N1—C10—C9	119.2 (2)
O21—C2—C3	123.8 (2)	C5—C10—C9	120.5 (2)
N1—C2—C3	117.00 (15)	C12—C11—C16	118.6 (2)
C4—C3—C2	122.4 (2)	C12—C11—N41	120.2 (2)
C3—C4—N41	123.4 (2)	C16—C11—N41	121.1 (2)
C3—C4—C5	119.2 (2)	C11—C12—C13	121.1 (2)
N41—C4—C5	117.42 (15)	C14—C13—C12	119.7 (2)
C4—N41—C11	123.7 (2)	O141—C14—C13	124.7 (2)
C6—C5—C10	117.9 (2)	O141—C14—C15	115.8 (2)
C6—C5—C4	124.6 (2)	C13—C14—C15	119.5 (2)
C10—C5—C4	117.49 (15)	C14—O141—C17	117.59 (14)
C7—C6—C5	121.2 (2)	C16—C15—C14	120.2 (2)
C6—C7—C8	120.3 (2)	C15—C16—C11	120.8 (2)
C9—C8—C7	120.0 (2)	O141—C17—C18	107.2 (2)
C8—C9—C10	120.1 (2)		

H atoms were refined isotropically; the C—H bond lengths are in the range 0.90–1.02 Å.

Data collection: *CAD*-4 *Software* (Enraf–Nonius, 1989); cell refinement: *CAD*-4 *Software*; data reduction: *WinGX*98 (Farrugia, 1998*a*); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*-3 (Farrugia, 1998*b*); software used to prepare material for publication: *SHELXL*97.

The authors are indebted to the Russian Foundation for Basic Research for covering the licence fee for use of the Cambridge Structural Database (project 99–07–90133).

References

Enraf–Nonius (1989). CAD-4 *Software*. Version 5.0. Enraf–Nonius, Delft, The Netherlands.
Farrugia, L. J. (1998*a*). *WinGX*98. University of Glasgow, Scotland.
Farrugia, L. J. (1998*b*). *ORTEP*3 for Windows. University of Glasgow, Scotland.
Kurzer, F. & Douraghi-Zaden, K. (1967). *Chem. Rev.* **67**, 107–152.
Sheldrick, G. M. (1997). *SHELXL*97 and *SHELXS*97. University of Göttingen, Germany.