Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methyl-2-(8-quinolyl)phthalazin-1-one

Daniel E. Lynch[a]* and Ian McClenaghan[b]

[a]School of Science and the Environment, Coventry University, Coventry CV1 5FB, England, and [b]Key Organics Ltd, Highfield Industrial Estate, Camelford, Cornwall PL32 9QZ, England

Correspondence e-mail: apx106@coventry.ac.uk

Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.004 Å
R factor = 0.056
wR factor = 0.179
Data-to-parameter ratio = 15.0

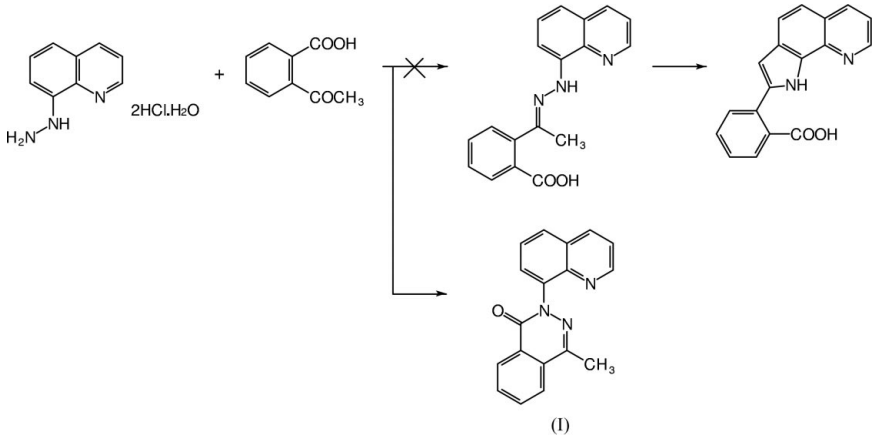
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The structure of the title compound, $C_{18}H_{13}N_3O$, comprises a twisted molecule, with the dihedral angle between the two ring systems being 72.4 (1)°. The phthalazin-1-one O atom has three C—H···O close contacts.

Received 23 August 2002
Accepted 27 August 2002
Online 6 September 2002

Comment

The title compound, (I) (Fig. 1), was obtained, rather than the intermediate hydrazone, from the reaction of 8-hydrazinoquinoline dihydrochloride hydrate and 2-acetylbenzoic acid, as shown in the reaction scheme below.



(I)

The intended product, the (*E*)-1-ethanone 8-quinolylhydrozone derivative (for example, Lynch & McClenaghan, 2001*a*), might have been useful in the cyclization to the

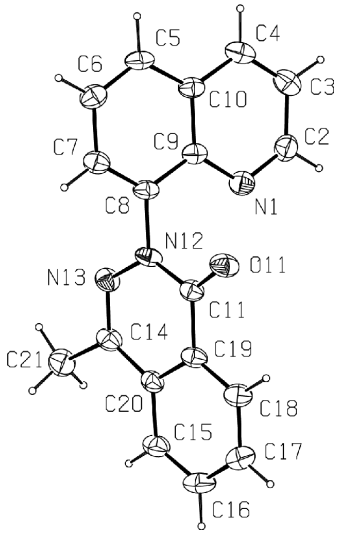


Figure 1
The molecular configuration and atom-numbering scheme for the title compound, showing 50% probability ellipsoids.

corresponding pyrrolo[3,2-*h*]quinoline (for example, Lynch & McClenaghan, 2001*b*). However, products similar to (I) have been reported for the reactions of phenylhydrazine with, respectively, 2-acetylbenzoic acid (Rowe & Peters, 1931), 2-acetylbenzonitrile (Helberger & Rebay, 1937), and 3-(2-carboxyphenyl)-3-oxo-propionic acid (Roser, 1885). In (I), the two rings are inclined at 72.4 (1)° and the phthalazin-1-one O atom has three C—H···O close contacts (Table 1).

Experimental

8-Hydrazinoquinoline dihydrochloride hydrate (0.03 mmol), 2-acetylbenzoic acid (0.03 mmol) and triethylamine (0.046 mmol) were refluxed in 1:5 aqueous ethanol for 80 min. A crystalline solid was collected following acidification with dilute acetic acid (yield 95%). Crystals were grown from an ethanol solution (m.p. 450–452 K).

Crystal data

$C_{18}H_{13}N_3O$
$M_r = 287.31$
Triclinic, $P\overline{1}$
$a = 7.9530\ (4)$ Å
$b = 8.4914\ (6)$ Å
$c = 10.8850\ (7)$ Å
$\alpha = 77.060\ (6)°$
$\beta = 74.114\ (5)°$
$\gamma = 86.277\ (3)°$
$V = 689.05\ (7)$ Å^3
$Z = 2$
$D_x = 1.385$ Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 6981 reflections
$\theta = 2.9$–$27.5°$
$\mu = 0.09$ mm^{-1}
$T = 150\ (2)$ K
Block, colourless
0.10 × 0.10 × 0.05 mm

Data collection

Bruker–Nonius KappaCCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
$T_{min} = 0.991$, $T_{max} = 0.996$
9188 measured reflections
3005 independent reflections
1507 reflections with $I > 2\sigma(I)$
$R_{int} = 0.075$
$\theta_{max} = 27.4°$
$h = -10 \rightarrow 10$
$k = -10 \rightarrow 10$
$l = -12 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.179$
$S = 0.97$
3005 reflections
200 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0888P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.30$ e Å^{-3}
$\Delta\rho_{min} = -0.30$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O11^{i}	0.95	2.57	3.442 (3)	153
C16—H16···N1^{ii}	0.95	2.60	3.469 (4)	153
C21—H21···O11^{iii}	0.98	2.36	3.194 (3)	142

Symmetry codes: (i) $x, y-1, z$; (ii) $1-x, 1-y, 1-z$; (iii) $1+x, y, z$.

All H atoms were included in the refinement, at calculated positions, as riding models, with C—H distances set to 0.95 (Ar-H) or 0.98 Å (CH_3).

Data collection: *DENZO* (Otwinowski & Minor, 1997) and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *PLATON*97 (Spek, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Helberger, J. H. & von Rebay, A. (1937). *Justus Liebigs Ann. Chem.* **531**, 279–287.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Lynch, D. E. & McClenaghan, I. (2001*a*). *Acta Cryst.* E**57**, o52–o53.
Lynch, D. E. & McClenaghan, I. (2001*b*). *Acta Cryst.* E**57**, o56–o57.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Roser, W. (1885). *Chem. Ber.* **18**, 804.
Rowe, F. M. & Peters, A. T. (1931). *J. Chem. Soc.* pp. 1918–1925.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.
Spek, A. L. (1997). *PLATON*97. Version of May 1997. University of Utrecht, The Netherlands.