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# 2-(Quinolin-8-yloxy)benzoic acid

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In the title compound, $C_{16}H_{11}NO_3$, the quinolin-8-yloxy and 2-carboxyphenyl groups are linked through an ether O atom, the angle at this atom being 116.4 (1)° in one molecule and 114.8 (1)° in the other independent molecule. In both molecules, the carboxylic acid group interacts with the heterocyclic moiety through an intramolecular hydrogen bond.

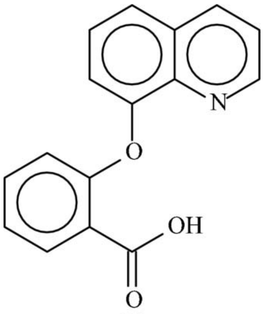
**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.002 Å
$R$ factor = 0.042
$wR$ factor = 0.120
Data-to-parameter ratio = 14.3

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

## Comment

The title compound, (I), was designed as a chelating ligand as it has a nitrogen site from the quinolinyl ring system, an ether linkage, and a carboxyl unit on the benzoic acid portion of the molecule. The chemical literature has not documented this compound yet, as no entries were uncovered by SciFinder (American Chemical Society, 2006). The 4-(quinolin-8-oyl)-benzoic acid isomer is claimed as a drug for treating some diseases (Letourneau *et al.*, 2005) but the position of the carboxyl substituent is unsuitable for the purpose of preparing coordination compounds.



(I)

The asymmetric unit contains two molecules. The molecule of (I) consists of a quinolinyl and a carboxyphenyl unit that are linked through an ether O atom. The angle at this atom is 116.4 (1)° in one molecule and 114.8 (1)° in the other independent molecule (Fig. 1). In both molecules, the carboxylic acid group interacts with the heterocyclic system through an intramolecular hydrogen bond (Table 1). The formation of the hydrogen bond is partially facilitated by a twisting of the aromatic ring with respect to the heterocycle [the twist angle is 69.4 (1)° for the molecule with the larger ether angle, and 74.5 (1)° for the molecule with the smaller ether angle].

## Experimental

A mixture of 2-iodobenzoic acid (2.48 g, 10 mmol), 8-hydroxyquinoline (1.45 g, 10 mmol), potassium carbonate (2.76 g, 20 mmol), copper powder (0.13 g, 2 mmol), copper(I) iodide (0.38 g, 3 mmol) and *n*-amyl alcohol (20 ml) was heated at 433 K for 2 h. The mixture was cooled and water added; the insoluble material was removed by filtration. The filtrate was acidified with dilute hydrochloric acid and the solid that separated was collected (1.50 g, 60% yield; m.p. 450 K). Yellow single crystals of (I) were obtained by using methanol as solvent for recrystallization.

*Crystal data*

$C_{16}H_{11}NO_3$
$M_r = 265.26$
Triclinic, $P\bar{1}$
$a = 8.2123$ (5) Å
$b = 10.2704$ (6) Å
$c = 15.6104$ (9) Å
$\alpha = 84.265$ (1)°
$\beta = 85.629$ (1)°
$\gamma = 69.425$ (1)°
$V = 1225.3$ (1) Å$^3$
$Z = 4$
$D_x = 1.438$ Mg m$^{-3}$
Mo $K\alpha$ radiation
$\mu = 0.10$ mm$^{-1}$
$T = 293$ (2) K
Block, yellow
0.48 × 0.32 × 0.22 mm

*Data collection*

Bruker SMART 1K area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: none
10403 measured reflections
5271 independent reflections
3532 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.023$
$\theta_{\rm max} = 27.1°$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.042$
$wR(F^2) = 0.120$
$S = 1.03$
5271 reflections
369 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0672P)^2 + 0.0304P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\rm max} = 0.001$
$\Delta\rho_{\rm max} = 0.25$ e Å$^{-3}$
$\Delta\rho_{\rm min} = -0.22$ e Å$^{-3}$

**Table 1**
Hydrogen-bond geometry (Å, °).

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1*o*···N1 | 0.87 (1) | 1.81 (1) | 2.668 (2) | 169 (2) |
| O5—H5*o*···N2 | 0.87 (1) | 1.82 (1) | 2.683 (2) | 171 (2) |

Carbon-bound H atoms were placed at calculated positions (C—H = 0.93 Å) and were included in the refinement in the riding model approximation, with $U_{\rm iso}$(H) set to 1.2 times $U_{\rm eq}$(C). The acid H atoms were located in a difference Fourier map, and were refined with the distance restraint O—H = 0.85 (1) Å; their displacement parameters were freely refined.

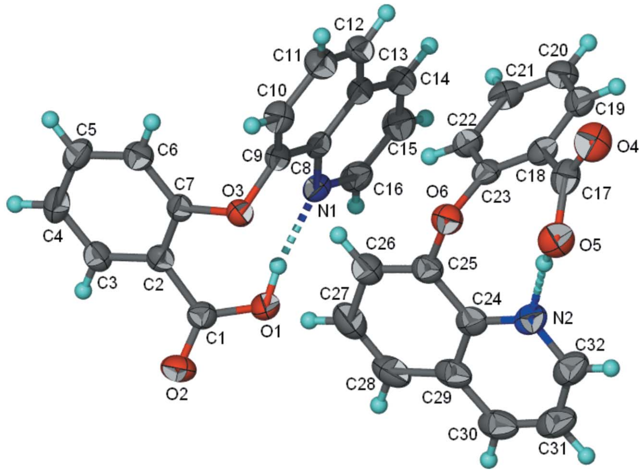


**Figure 1**
The asymmetric unit of (I). Displacement ellipsoids are drawn at the 70% probability level, and H atoms as spheres of arbitrary radii. The dashed lines denote the intramolecular hydrogen bonds.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *SHELXL97* and *publCIF* (Westrip, 2006).

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