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# 2-Aminoquinolin-8-yl *p*-toluenesulfonate

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The essentially planar quinoline fragment and the aromatic ring of the toluenesulfonate group of the title compound, $C_{16}H_{14}N_2O_3S$, form a dihedral angle of 52.2 (1)°; the torsion angle about the central bridge C—O—S—C is −69.3 (2)°. The N—H···N and N—H···O hydrogen bonds, involving the H atoms of the amino group and the quinoline and sulfonyl N and O atoms [N···N = 3.055 (3) Å and N···O = 3.058 (2) Å], link the molecules into dimers; a C—H···O interaction formed by the CH group in position 4 of the quinoline group [C···O = 3.293 (3) Å] further links the dimers into infinite chains running along the diagonal of the *ab* plane.

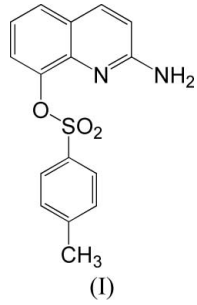
**Key indicators**

Single-crystal X-ray study
*T* = 299 K
Mean σ(C–C) = 0.004 Å
*R* factor = 0.042
*wR* factor = 0.119
Data-to-parameter ratio = 11.3

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

## Comment

8-Hydroxyquinoline derivatives show a wide spectrum of properties as analytical reagents, owing to their ability to form complexes with many metal ions (Bratzel *et al.*, 1972). In addition, 8-hydroxyquinoline (8-HQ) has received continuous attention as a platform for the construction of a number of selective and efficient fluoroionophores (Youk *et al.*, 2004). Although 8-HQ itself shows very low quantum yield in aqueous or organic solutions, many of its chelate metal complexes exhibit intense fluorescence (Song *et al.*, 2006). The selectivity of 8-HQ and its simple derivatives with respect to metal ions is rather poor, but it can be improved by appropriate substitution on the phenol O atom or aromatic rings. Moreover, organic fluorophores have received much attention in recent years, because of their numerous applications in the optoelectronics industry, as well as in the treatment of neurodegenerative diseases (Ooyama *et al.*, 2005; Raman *et al.*, 2005). As part of our ongoing search for new lead compounds based on the quinoline system, as potential fluorophores for Alzheimer's disease (da Silva *et al.*, 2005*a*,*b*,*c*,*d*,*e*), we undertook an X-ray diffraction study of the title compound, (I).




(I)

In the molecule of (I) (Fig. 1), the quinoline ring system, along with the amino group, is nearly planar, with maximum

deviations from the mean plane of −0.053 (2) Å for atom C9 and 0.070 (2) Å for atom N2; the plane of the aromatic ring of the toluenesulfonate group forms a dihedral angle of 52.2 (1)° with the aminoquinoline plane, and the C1—O3—S1—C10 torsion angle is −69.3 (2)°.

The N2—H21*N*···N1$^{i}$ and N2—H22*N*···O1$^{i}$ hydrogen bonds (Table 1) link the molecules in the structure into dimeric aggregates, which are further linked into infinite chains along the diagonal of the *ab* plane *via* the C6—H6···O1$^{ii}$ interactions (Fig. 2).

## Experimental

2-Amino-8-hydroxyquinoline (50 mg, 0.31 mmol) and *p*-toluenesulfonyl chloride (65.4 mg, 0.34 mmol) were dissolved in pyridine (2 ml) at 273 K with stirring and left to stand overnight. The mixture was then poured on to ice, filtered and washed with water. Single crystals suitable for X-ray data collection were obtained by recrystallization of the crude product (84 mg) from a methanol–dichloromethane (1:1) solution of (I). The product (yield 85%) was a colourless solid; m.p. 478 K.

### *Crystal data*

$C_{16}H_{14}N_2O_3S$
$M_r$ = 314.35
Triclinic, $P\overline{1}$
$a$ = 8.334 (1) Å
$b$ = 8.636 (1) Å
$c$ = 11.805 (1) Å
$\alpha$ = 96.35 (1)°
$\beta$ = 110.23 (1)°
$\gamma$ = 106.90 (1)°
$V$ = 741.40 (16) Å$^3$
$Z$ = 2
$D_x$ = 1.408 Mg m$^{-3}$
Cu $K\alpha$ radiation
$\mu$ = 2.07 mm$^{-1}$
$T$ = 299 (2) K
Prism, colourless
0.30 × 0.25 × 0.15 mm

### *Data collection*

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.601, $T_{max}$ = 0.739
2829 measured reflections
2632 independent reflections
2178 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.012
$\theta_{max}$ = 66.9°
3 standard reflections
frequency: 120 min
intensity decay: 1.5%

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.119
$S$ = 1.04
2632 reflections
232 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0732P)^2 + 0.1575P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.017
$\Delta\rho_{max}$ = 0.19 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.38 e Å$^{-3}$

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H21*N*···N1$^{i}$ | 0.99 (3) | 2.06 (3) | 3.055 (3) | 178 (2) |
| N2—H22*N*···O1$^{i}$ | 0.84 (3) | 2.35 (3) | 3.058 (2) | 143 (3) |
| C6—H6···O1$^{ii}$ | 0.94 (3) | 2.58 (3) | 3.293 (3) | 133 (2) |

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

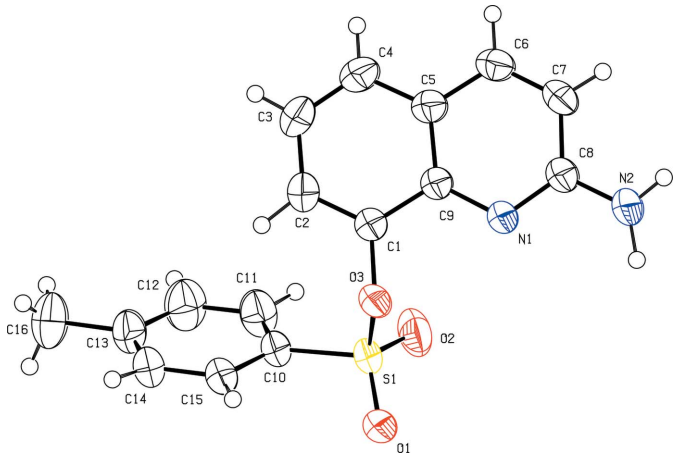



**Figure 1**
Molecular structure of (I), showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

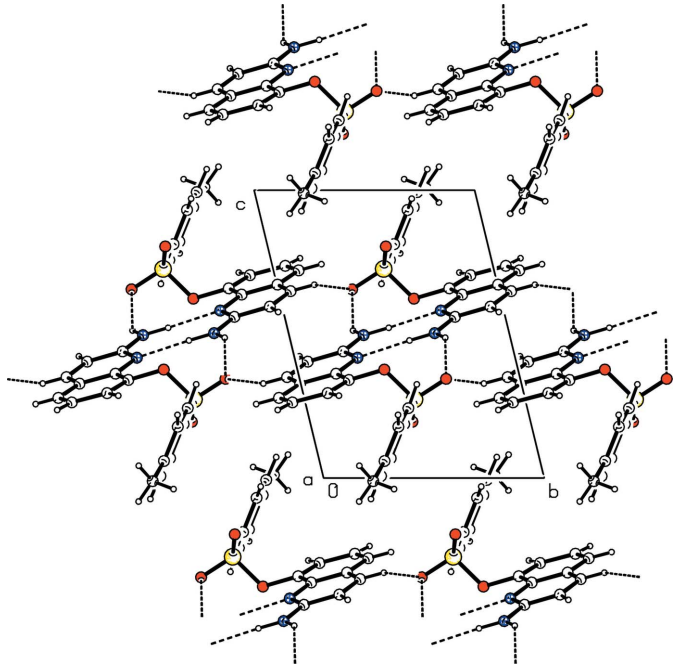



**Figure 2**
Molecular packing of (I), viewed approximately along the *a* axis, with hydrogen bonds shown as dashed lines.

The H atoms of the methyl group were placed in calculated positions and included in the refinement in a riding model approximation [C—H = 0.96 Å, $U_{iso}$(H) = 1.2$U_{eq}$(C)]. All other H atoms were located in a difference map, and their positional parameters were refined [C—H = 0.88 (3)–0.97 (3) Å, N—H = 0.84 (3) and 0.99 (3) Å], whereas their isotropic displacement parameters were set to 1.2$U_{eq}$ of the parent atom.

Data collection: *CAD-4-PC* Software (Enraf–Nonius, 1996); cell refinement: *CAD-4-PC* Software; data reduction: *REDU4* (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

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## References

Bratzel, M. P., Aaron, J. J., Winefordner, J. D., Schulman, S. G. & Gershon, H. (1972). *Anal. Chem.* **44**, 1240–1245.
Enraf–Nonius (1996). *CAD-4-PC Software*. Version 2.0. Nonius GmbH, Solingen, Germany.
North, A. C. T., Phillips, D. C. & Mathews, F. S. (1968). *Acta Cryst.* A**24**, 351–359.
Ooyama, Y., Nakamura, T. & Yoshida, K. (2005). *New J. Chem.* **29**, 447–456.
Raman, B., Ban, T., Yamaguchi, K., Sakai, M., Kawai, T., Naiki, H. & Goto, Y. (2005). *J. Biol. Chem.* **280**, 16157–16162.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*a*). *Acta Cryst.* E**61**, o3435–o3436.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*b*). *Acta Cryst.* E**61**, o3778–o3779.
Silva, L. E. da, Joussef, A. C., Foro, S. & Schmidt, B. (2005*c*). *Acta Cryst.* E**61**, o3780–o3781.
da Silva, L. E., Joussef, A. C., Foro, S. & Schmidt, B. (2005*d*). *Acta Cryst.* E**61**, o3837–o3838.
da Silva, L. E., Joussef, A. C., Foro, S. & Schmidt, B. (2005*e*). *Acta Cryst.* E**61**, o3782–o3783.
Song, K. C., Kim, J. S., Park, S. M., Chung, K.-C., Ahn, S. & Chang, S.-K. (2006). *Org. Lett.* **8**, 3413–3416.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Stoe & Cie (1987). *REDU4*. Version 6.2c. Stoe & Cie GmbH, Darmstadt, Germany.
Youk, J.-S., Kim, Y. H., Kim, E.-J., Youn, N. J. & Chang, S.-K. (2004). *Bull. Korean Chem. Soc.* **25**, 869–872.