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4-Nitro-*N*-(8-quinolyl)benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.005 Å
R factor = 0.055
wR factor = 0.150
Data-to-parameter ratio = 10.1

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

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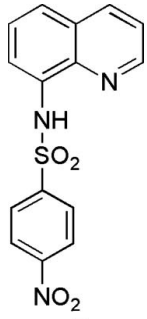
In the title compound, $C_{15}H_{11}N_3O_4S$, the dihedral angle between the quinoline ring system and the benzene ring is 79.9 (3)°. Intermolecular hydrogen bonds of types N—H···O, C—H···O and C—H···N are observed.

Comment

Zinc(II)-specific fluorophores are of substantial importance in the study of intracellular Zn^{2+}. Many zinquin-related fluorophore esters based on an 8-*p*-toluenesulfonamidoquinoline system have recently been developed and their properties investigated (Kimber *et al.*, 2003). We report here the structure of the title compound, (I), determined as a part of our studies to investigate potential new fluorophores to be used as ligands for coordination to Zn^{II} and Cu^{II} ions. The key feature of the molecular structure of (I) (Fig. 1) is the C1—N1—S1—C10 dihedral angle of 79.9 (3)°, *i.e.* that formed between the phenyl ring and the quinoline group. The crystal packing of (I) is stabilized through a hydrogen-bonding network, as shown in Fig. 2 and detailed in Table 1.



(I)

Experimental

Compound (I) was prepared by the overnight reaction of one equivalent of 8-aminoquinoline and a 1.1 equivalent of *p*-nitrobenzenesulfonyl chloride in the presence of pyridine, according to the literature procedure of Kimber *et al.* (2000). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from a methanol-dichloromethane (1:1) solution of (I).

Crystal data

$C_{15}H_{11}N_3O_4S$
M_r = 329.33
Monoclinic, $P2_1$
a = 5.0135 (6) Å
b = 20.636 (2) Å
c = 6.966 (1) Å
β = 99.28 (1)°
V = 711.26 (15) Å^3
Z = 2
D_x = 1.538 Mg m^{-3}
Cu *Kα* radiation
Cell parameters from 25 reflections
θ = 4.3–20.3°
μ = 2.27 mm^{-1}
T = 299 (2) K
Needle, colorless
0.60 × 0.18 × 0.10 mm

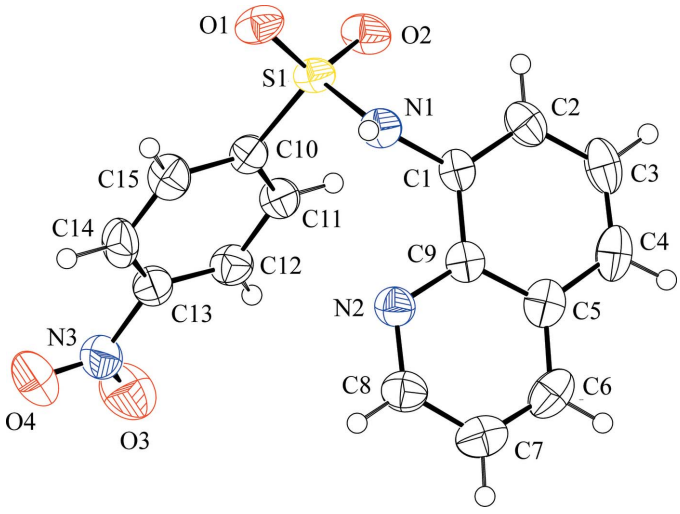


Figure 1
Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

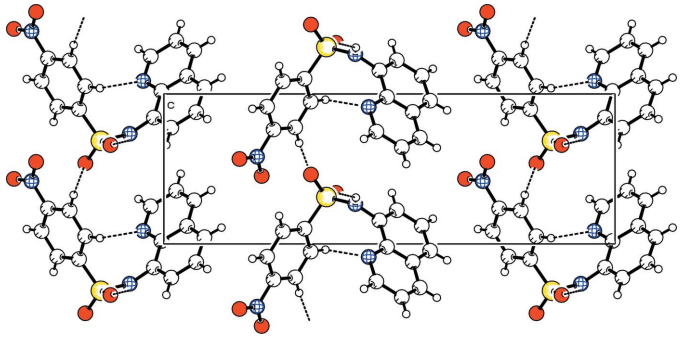


Figure 2
Molecular packing of (I), with hydrogen bonds shown as dashed lines.

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.282, T_{max} = 0.792
2347 measured reflections
2109 independent reflections
2081 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 67.9°
$h = -6 \rightarrow 0$
$k = -24 \rightarrow 11$
$l = -8 \rightarrow 8$
3 standard reflections
frequency: 120 min
intensity decay: 1.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.150
S = 1.14
2109 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1304P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.35 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.024 (3)
Absolute structure: Flack (1983), 778 Friedel pairs
Flack parameter: 0.05 (2)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O2^{i}	0.86	2.16	2.935 (4)	150
C11—H11···N2^{ii}	0.93	2.50	3.407 (5)	1
C12—H12···O1^{iii}	0.93	2.45	3.360 (4)	166

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

The H atoms were included in the riding-model approximation, with N—H = 0.86 Å and C—H = 0.93 Å, and with U_{iso}(H) = $1.2U_{eq}$(N,C).

Data collection: *CAD-4/PC Software* (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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