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N-(6-Methoxy-2-methyl-8-quinolyl)-4-*n*-propylbenzenesulfonamide

Luiz Everson da Silva,[a,b] Antonio Carlos Joussef,[a] Sabine Foro[b]* and Boris Schmidt[b]

[a]Departamento de Química–UFSC, 88040-900 Florianópolis, SC, Brazil, and [b]Clemens Schöpf-Institut für Organische Chemie und Biochemie, Technische Universität Darmstadt, Petersenstrasse 22, D-64287 Darmstadt, Germany

Correspondence e-mail: foro@tu-darmstadt.de

Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.004 Å
R factor = 0.046
wR factor = 0.131
Data-to-parameter ratio = 12.5

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

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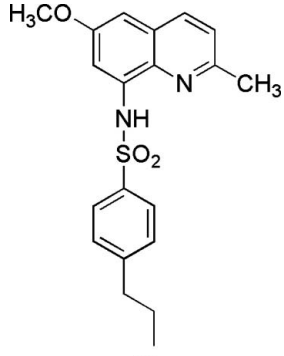
In the title compound, $C_{20}H_{22}N_2O_3S$, the torsion angle about the N—S bond between the quinoline system and the benzene ring is −48.7 (2)°. An intramolecular N—H···N and an intermolecular C—H···O hydrogen bond are observed in the crystal structure.

Comment

Various fluorescence-based zinc probes have been developed. Some of these are fluorescent adducts of Zn-chelating peptides and proteins, while others are dye adducts of Zn-chelating macrocyclic compounds. Zinc chelators based on a quinoline core, such as 6-methoxy-(8-*p*-toluenesulfonamide)quinoline (TSQ), are currently the most widely used zinc-activated fluorophores (Fahrni & O'Halloran, 1999). As part of our continuing study of 8-aminoquinolinesulfonamide derivatives capable of binding Zn^{2+} (da Silva *et al.*, 2005*a*,*b*,*c*,*d*,*e*, 2006), the structure of the title compound (I), was determined.



(I)

The C1—N1—S1—C10 torsion angle is −48.7 (2)°. The NH group forms an intramolecular hydrogen bond to the quinoline N atom. In addition, there is an intermolecular C—H···O hydrogen bond. The three-dimensional network is shown in the packing diagram (Fig. 2) and details are given in Table 1.

Experimental

Compound (I) was prepared according to the literature procedure of Kimber *et al.* (2003). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from methanol–dichloromethane (1:1 *v*/*v*).

Crystal data

$C_{20}H_{22}N_2O_3S$
M_r = 370.46
Triclinic, $P\overline{1}$
a = 8.4437 (8) Å
b = 9.7548 (8) Å
c = 12.1870 (8) Å
α = 95.254 (6)°
β = 94.757 (7)°
γ = 103.426 (8)°
V = 966.62 (14) Å^3
Z = 2
D_x = 1.273 Mg m^{-3}
Cu $K\alpha$ radiation
Cell parameters from 25 reflections
θ = 4.7–22.8°
μ = 1.66 mm^{-1}
T = 299 (2) K
Plate, light brown
0.30 × 0.28 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.697, T_{max} = 0.847
4198 measured reflections
3438 independent reflections
2585 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 66.9°
$h = -10 \rightarrow 1$
$k = -11 \rightarrow 11$
$l = -14 \rightarrow 14$
3 standard reflections
frequency: 120 min
intensity decay: 1.0%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.131
S = 1.04
3438 reflections
274 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.1977P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.006
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H20···N2	0.86 (3)	2.12 (3)	2.639 (3)	119 (2)
C6—H6···O1^{i}	0.95 (3)	2.51 (3)	3.356 (3)	149 (2)

Symmetry code: (i) $x, y-1, z$.

The H atoms of the CH_3 groups were positioned with idealized geometry and refined using a riding model, with C—H = 0.96 Å and U_{iso}(H) = 1.2U_{eq}(C). All other H atoms were located in a difference map. Their coordinates were refined, but their isotropic displacement parameters were set at 1.2 times U_{eq} of the parent atom.

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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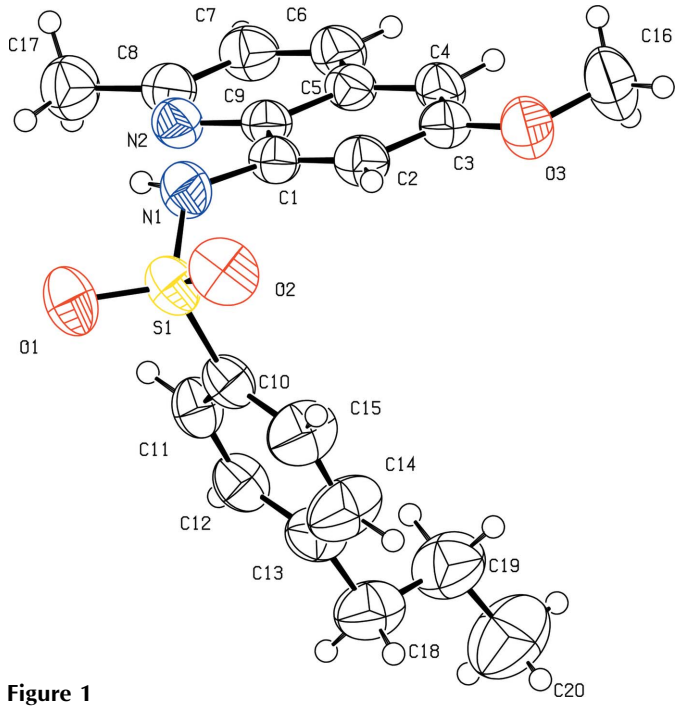

Figure 1
The molecular structure of (I), showing the atom labelling. Displacement ellipsoids are drawn at the 50% probability level.

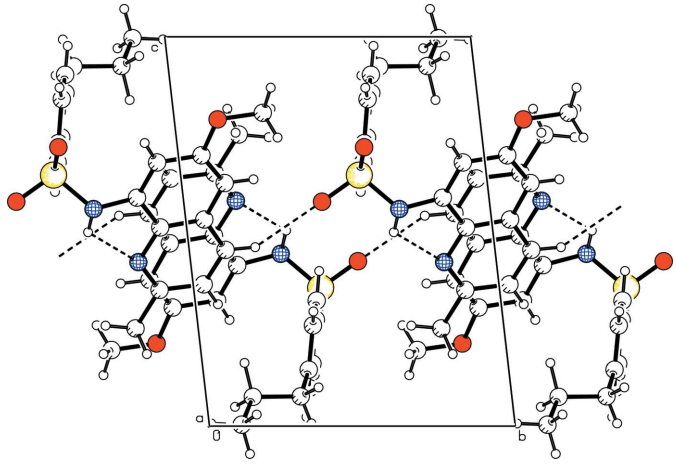

Figure 2
The molecular packing of (I) with hydrogen bonds shown as dashed lines.

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