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2-Aminoquinolin-8-yl 3,5-difluorobenzenesulfonate

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

[a]Universidale Federal de Mato Grosso–Departamento de Química–UFMT, 78060-900 Cuiabá, MT, 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) = 0.005 Å
R factor = 0.062
wR factor = 0.186
Data-to-parameter ratio = 11.6

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

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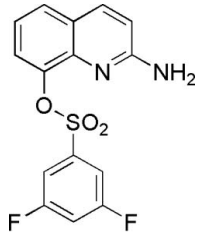
The molecular packing of the title compound, $C_{15}H_{10}F_2N_2O_3S$, is stabilized by a hydrogen-bonded network. Both H atoms of the amino group form intermolecular hydrogen bonds of types N—H···N [2.26 (5) Å] and N—H···O [2.30 (5) Å]. The nearly planar quinoline system and the aromatic ring of the toluenesulfonate group form a dihedral angle of 31.1 (6)°; the torsion angle about the central C—O—S—C bridge is −120.4 (2)°.

Comment

As part of our ongoing search for new lead compounds based on the quinoline system as a potential fluorophore for Alzheimer's disease (da Silva, Joussef *et al.*, 2007*a*,*b*; da Silva *et al.*, 2007), we have performed an investigation of the crystal structure of the title compound, (I).



(I)

The C1—O3—S1—C10 torsion angle of −120.4 (2)° illustrates the non-planarity of the molecule formed by the quinoline system with the benzene ring. The quinoline ring system, with the amino group, is nearly planar with maximum

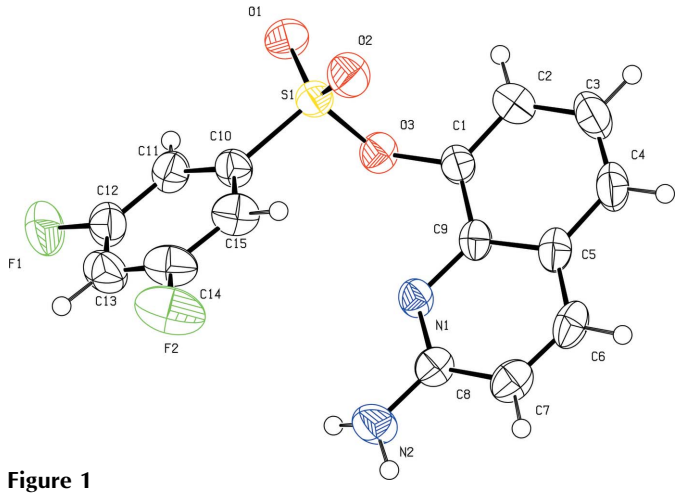


Figure 1
Molecular structure of (I), showing the atom labeling and displacement ellipsoids drawn at the 50% probability level.

deviations from the mean plane of −0.033 (3) Å for atom N1 and 0.043 (3) Å for atom C7; the plane of the aromatic ring of the toluenesulfonate group forms a dihedral angle of 31.1 (6)° with the aminoquinoline plane. The molecular packing of (I) is stabilized by hydrogen bonds (Table 1).

Experimental

The title compound was prepared according to the literature procedure of da Silva, Joussef *et al.* (2007*a*). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization of the crude product from a methanol–dichloromethane (1:1) solution of (I) (m.p. 440–441 K).

Crystal data

$C_{15}H_{10}F_2N_2O_3S$
M_r = 336.31
Triclinic, $P\overline{1}$
a = 7.7926 (7) Å
b = 9.253 (1) Å
c = 9.795 (1) Å
α = 90.233 (9)°
β = 96.787 (8)°
γ = 92.516 (8)°
V = 700.61 (12) Å^3
Z = 2
D_x = 1.594 Mg m^{-3}
Cu $K\alpha$ radiation
μ = 2.45 mm^{-1}
T = 299 (2) K
Plate, light brown
0.40 × 0.25 × 0.08 mm

Data collection

Nonius CAD-4 diffractometer
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.403, T_{max} = 0.711
(expected range = 0.466–0.822)
2699 measured reflections
2491 independent reflections
2028 reflections with $I > 2\sigma(I)$
R_{int} = 0.104
θ_{max} = 66.9°
3 standard reflections
frequency: 120 min
intensity decay: 1.5%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.187
S = 1.08
2491 reflections
215 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1277P)^2 + 0.1408P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.65 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.0070 (19)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H21N···N1^{i}	0.92 (5)	2.26 (5)	3.144 (4)	162 (4)
N2—H22N···O1^{ii}	0.82 (5)	2.30 (5)	3.062 (4)	156 (4)

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

The carbon-bound H atoms were positioned with idealized geometry using a riding model (C—H = 0.93 Å). The amino H atoms were located in a difference map and refined freely. All H atoms were refined with isotropic displacement parameters set to $1.2U_{eq}$ of the parent atom.

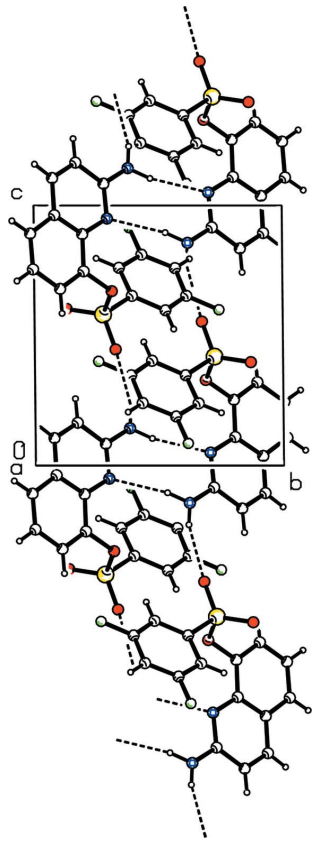


Figure 2
Molecular packing of (I) with hydrogen bonding shown as dashed lines.

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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