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2,4,6-Triisopropyl-*N*-(6-methoxy-2-methyl-8-quinolyl)benzenesulfonamide

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Key indicators

Single-crystal X-ray study
T = 299 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.152
Data-to-parameter ratio = 16.7

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

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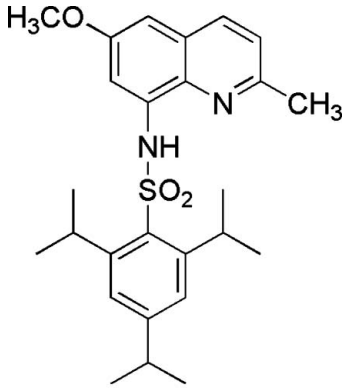
In the crystal structure of the title compound, $C_{26}H_{34}N_2O_3S$, the quinoline ring system, with methoxy and methyl substituents, is nearly planar. An intramolecular hydrogen bond [N—H···N = 2.16 (2) Å] is observed.

Comment

Biological imaging of specific molecules can provide direct information on molecular functions in living systems. The most important breakthrough is the creation of selective and sensitive molecules. Some of these sensor molecules, such as Zinquin ester analogues (Hendrickson *et al.*, 1997), have led to new findings about the role of Zn^{2+} in living systems. As part of our continuing study of the 8-aminoquinolinesulfonamide derivatives capable of binding Zn^{2+} (da Silva *et al.*, 2005*a*,*b*,*c*,*d*,*e*), the structure of the title compound, (I), was determined.



(I)

The key feature of the molecular structure of (I) (Fig. 1) is the C1—N1—S1—C10 torsion angle of 62.3 (2)°, which illustrates the non-planarity of the molecule. The quinoline ring system, with methoxy and methyl substituents, is nearly planar, with maximum deviations from the mean plane of −0.032 (2) Å for atom C9 and 0.042 (2) Å for atom C2.

The H atom of the NH group forms an intramolecular hydrogen bond to the quinoline N atom (Table 1 and Fig. 2).

Experimental

Compound (I) was prepared according to the procedure described by Kimber *et al.* (2003). Single crystals of (I) suitable for X-ray data collection were obtained by recrystallization from a methanol–dichloromethane (1:1) solvent mixture (m.p. 460–461 K; yield 57%).

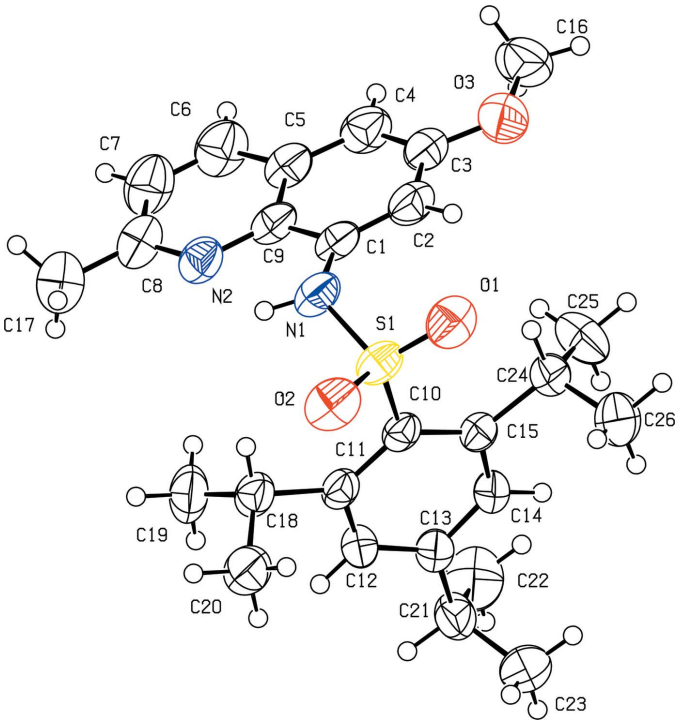


Figure 1
The molecular structure of (I), showing the atom-labelling and with displacement ellipsoids drawn at the 50% probability level.

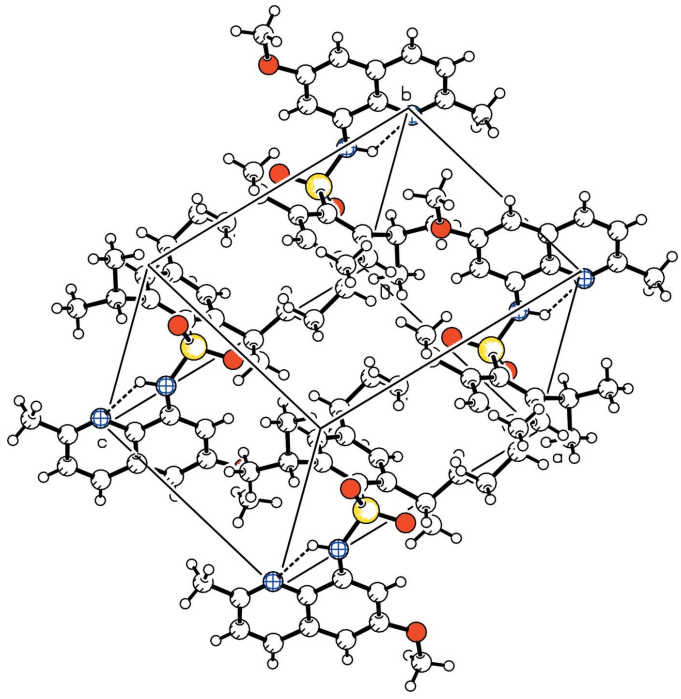


Figure 2
The crystal packing of (I), with hydrogen bonds shown as dashed lines.

Crystal data

$C_{26}H_{34}N_2O_3S$
M_r = 454.61
Triclinic, $P\overline{1}$
a = 9.1402 (8) Å
b = 11.7266 (9) Å
c = 11.8755 (9) Å
α = 83.329 (6)°
β = 89.061 (7)°
γ = 78.543 (7)°
V = 1239.02 (17) Å^3
Z = 2
D_x = 1.219 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 2832 reflections
θ = 2.3–23.4°
μ = 0.16 mm^{-1}
T = 299 (2) K
Prism, colourless
0.45 × 0.44 × 0.30 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with Sapphire CCD area detector
ω and φ scans
Absorption correction: analytical *CrysAlis RED* (Oxford Diffraction, 2002)
T_{min} = 0.914, T_{max} = 0.962
10522 measured reflections
4896 independent reflections
3152 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 26.4°
$h = -11 \rightarrow 7$
$k = -14 \rightarrow 14$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.152
S = 0.98
4896 reflections
293 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.092P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.013
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···N2	0.91 (2)	2.16 (2)	2.667 (3)	114 (2)

The H atom of the NH group was located in a difference map and refined freely. All other H atoms were positioned with idealized geometry using a riding model, with C—H = 0.93 (aromatic), 0.98 (methine) and 0.96 Å (methyl). All H atoms were refined with U_{iso}(H) = 1.2U_{eq}(parent atom).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2002); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2002); data reduction: *CrysAlis RED*; 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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