Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′-Bis(4-fluoroanilino)-3,3′-(3,6-dioxaoctane-1,8-diyl)diquinazolin-4(3*H*)-one

Xiang Wang,[a]* Zuan Ma[b] and Yu-Lu Chen[c]

[a]Department of Chemistry, Kaili College, Guizhou 556000, People's Republic of China, [b]Department of Medicinal Chemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China, and [c]Department of Chemistry, Xianning Vocational and Technical College, Xianning 437100, People's Republic of China
Correspondence e-mail: wangx0828@sina.com

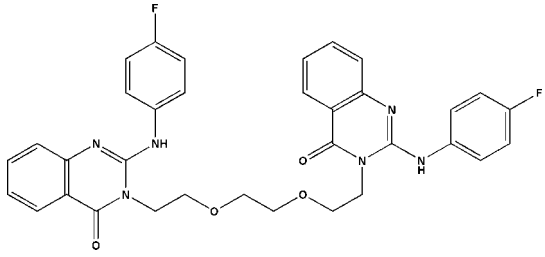
Received 10 November 2008; accepted 3 December 2008

Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.048; wR factor = 0.146; data-to-parameter ratio = 13.6.

In the centrosymmetric title compound, $C_{34}H_{30}F_2N_6O_4$, the dihedral angle between the quinazolinone and fluorobenzene ring planes are 71.00 (2) and 74.94 (2)° and an intramolecular N—H···O interaction stabilizes the conformation. In the crystal, C—H···F and C—H···O links help to establish the packing.

Related literature

For the biological activity of quinazolinones, see: Shiba *et al.* (1997); Ding *et al.*, 2004. For the crystal structures of other fused heterocyclic derivatives, see: Wang *et al.* (2006); Xu *et al.* (2006).



Experimental

Crystal data

$C_{34}H_{30}F_2N_6O_4$
M_r = 624.64
Monoclinic, $C2/c$
a = 13.923 (3) Å
b = 12.509 (3) Å
c = 18.726 (4) Å
β = 97.08 (3)°
V = 3236.6 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 (2) K
0.20 × 0.10 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.982, T_{max} = 0.991
2834 measured reflections
2834 independent reflections
2263 reflections with $I > 2\sigma(I)$
R_{int} = 0.0123

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.146
S = 1.06
2834 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2	0.86	2.18	2.7954 (19)	128
C16—H16A···F1^{i}	0.97	2.54	3.388 (2)	146
C16—H16B···O1^{ii}	0.97	2.43	3.377 (2)	164

Symmetry codes: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, -y+1, -z+1$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

We thank Dr Xiang-Gao Meng for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2676).

References

Bruker (2001). *SMART* and *SAINT-Plus* . Bruker AXS Inc., Madison, Wisconsin, USA.
Ding, M. W., Chen, Y. F. & Huang, N. Y. (2004). *Eur. J. Org. Chem.* pp. 3872–3878.
Sheldrick, G. M. (2003). *SADABS*. Bruker AXS,inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Shiba, S. A., El-Khamry, A. A., Shaban, M. E. & Atia, K. S. (1997). *Pharmazie*, **52**, 189–194.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Wang, X., Zheng, A.-H. & Xu, S.-Z. (2006). *Acta Cryst.* E**62**, o4791–o4792.
Xu, S.-Z., Hu, Y.-G., Wang, X. & Ding, M.-W. (2006). *Acta Cryst.* E**62**, o2229–o2230.