Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

7-(4-Fluorophenyl)-8*H*-benzo[*h*]indeno-[1,2-*b*]quinolin-8-one

Shu-Jiang Tu,* Yan Zhang and Run-Hong Jia

Department of Chemistry, Xuzhou Normal University, Xuzhou 221116, People's Republic of China

Correspondence e-mail: laotu2001@263.net

Received 12 August 2006
Accepted 15 August 2006

The title compound, $C_{26}H_{14}FNO$, was synthesized by the reaction of 4-fluorobenzaldehyde, 1-naphthylamine and 1,3-indanedione in glycol under microwave irradiation. The fused ring system is approximately planar and the attached fluorophenyl ring forms a dihedral angle of 65.21 (8)°. The molecules are linked by intermolecular C—H···O hydrogen bonds and π–π interactions, forming a chain structure

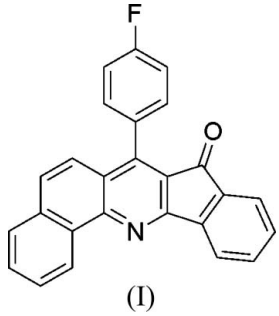
Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.005 Å
R factor = 0.039
wR factor = 0.089
Data-to-parameter ratio = 6.7

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

Comment

Indenoquinoline derivatives show a wide range of biological properties, such as 5-HT-receptor binding activity and anti-inflammatory activity (Lu *et al.*, 2003). They also act as anti-tumor agents, inhibitors for steroid reductase (Deady *et al.*, 2000), acetylcholinesterase inhibitors and anti-malarial agents (Rampa *et al.*, 2000). We report here the crystal structure of the title compound, (I).



(I)

The fused ring system containing the naphthalene, pyridine and indenone rings is approximately planar with an r.m.s. deviation of 0.045 Å (Fig. 1). The dihedral angle between the N1/O1/C1–C20 and C21–C26 planes is 65.21 (8)°.

The crystal structure of (I) is stabilized by intermolecular C—H···O hydrogen bonds (Table 1), and π–π stacking interactions involving the C1/C2/C7–C9 (centroid *Cg*1) and C11–C14/C19/C20 (centroid *Cg*2) rings, with a $Cg1\cdots Cg2^{iv}$ distance of 3.542 (3) Å [symmetry code: (iv) x, 1 + y, z], resulting in the formation of a chain structure along the *b* axis. In addition, a C—H···π interaction involving the C14–C19 benzene ring (centroid *Cg*3) is observed.

Experimental

Compound (I) was prepared by the reaction of 4-fluorobenzaldehyde (1 mmol), 1-naphthylamine (1 mmol) and 1,3-indanedione (1 mmol) in glycol (2 ml) under microwave irradiation for 3 min. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 93%; m.p. 573 K).

Crystal data

$C_{26}H_{14}FNO$
M_r = 375.38
Monoclinic, $P2_1$
a = 10.971 (4) Å
b = 6.274 (2) Å
c = 13.540 (4) Å
β = 103.115 (5)°
V = 907.7 (5) Å^3
Z = 2
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
Block, yellow
0.50 × 0.23 × 0.12 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.989
4768 measured reflections
1751 independent reflections
1130 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.089
S = 1.00
1751 reflections
262 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.039P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.12 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C6—H6···O1^{i}	0.93	2.44	3.365 (5)	173
C22—H22···O1^{ii}	0.93	2.34	3.237 (5)	163
C15—H15···*Cg*3^{iii}	0.93	2.88	3.685 (4)	146

Symmetry codes: (i) $-x, y+\frac{1}{2}, -z+1$; (ii) $x, y-1, z$; (iii) $-x+1, y-\frac{1}{2}, -z+2$. *Cg*3 is the centroid of the C14–C19 benzene ring.

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å and U_{iso}(H) = 1.2U_{eq}(C). In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

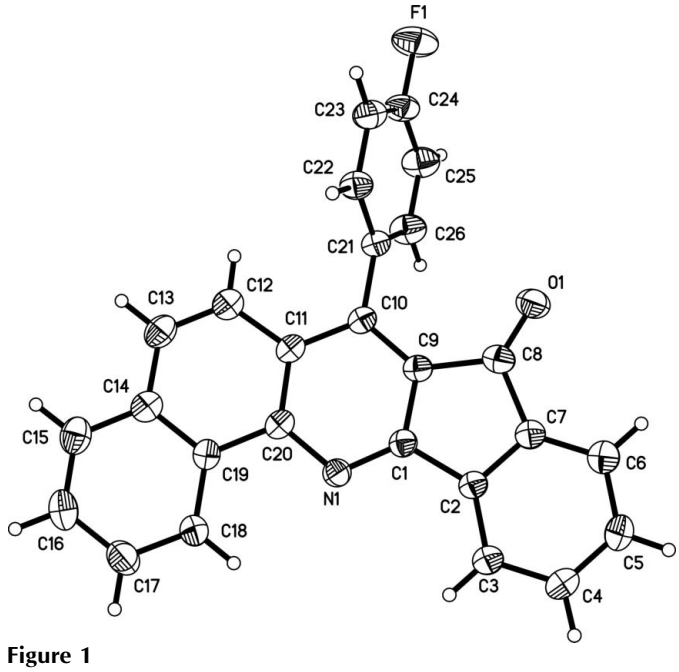


Figure 1
The structure of (I), showing 30% probability displacement ellipsoids.

The authors thank the National Natural Science Foundation of China (grant No. 20372057), the Open Foundation of the Key Laboratory of Organic Synthesis of Jiangsu Province, the College of Chemistry and Chemical Engineering, Suzhou University (grant No. JSK011), and the Key Laboratory of Biotechnology for Medicinal Plants of Jiangsu Province (grant No. 01AXL14) for financial support.

References

Bruker (1998). *SMART*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* and *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Deady, L. W., Desneves, J., Kaye, A. J., Finlay, G. J., Baguley, B. C. & Denny, W. A. (2000). *Bioorg. Med. Chem.* **8**, 977–984.
Lu, X., Petersen, J. L. & Wang, K. K. (2003). *Org. Lett.* **5**, 3277–3280.
Rampa, A., Bisi, A., Belluti, F., Gobbi, S., Valenti, P., Andrisano, V., Cavrini, V., Cavalli, A. & Recanatini, M. (2000). *Bioorg. Med. Chem.* **8**, 497–506.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.