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## Key indicators

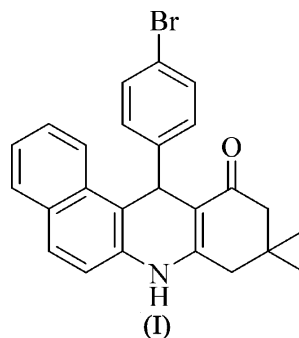
Single-crystal X-ray study  
 $T = 298\text{ K}$   
Mean  $\sigma(\text{C}-\text{C}) = 0.006\text{ \AA}$   
 $R$  factor = 0.044  
 $wR$  factor = 0.119  
Data-to-parameter ratio = 13.2For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.12-(4-Bromophenyl)-9,9-dimethyl-1,2,3,4,9,10-hexahydrobenz[*a*]acridin-11-one

The title compound,  $\text{C}_{25}\text{H}_{22}\text{BrNO}$ , has been synthesized by the reaction of 4-bromobenzaldehyde, 3,3-dimethylcyclopentane-1,3-dione with 2-naphthylamine in ethanol. In the crystal structure, the molecules are connected by  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds, forming chains along the  $a$  axis.

Received 13 April 2006  
Accepted 21 April 2006

## Comment

Many natural and synthetic compounds containing the acridine skeleton display interesting biological and physical activities, such as antimalaria (Nasim & Brychey, 1979; Thull & Testa, 1994; Reil *et al.*, 1994; Mandi *et al.*, 1994) and anti-tumour properties (Khurana *et al.*, 1990). Multihydroacridinone derivatives have been reported to have high fluorescence efficiencies and can be used as fluorescent molecular probes for the monitoring of polymerization processes (Popielarz *et al.*, 1997). Increasingly, they also receive attention due to the similarity of their properties with those of 1,4-dihydropyridines, which have similarities in structure with biologically important compounds, such as nicotinamide adenine dinucleotide (Srividya *et al.*, 1996). In this paper, we report the crystal structure of the title compound, (I).

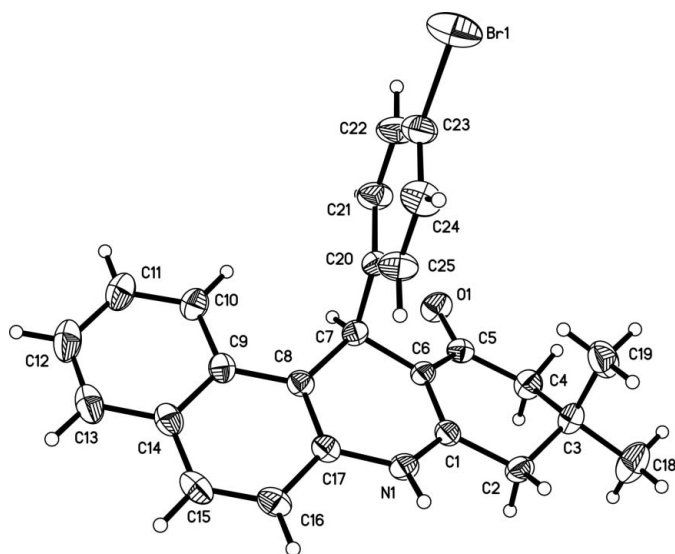


In compound (I), atoms C7 and N1 deviate from the C1/C6/C8/C17 plane by 0.321 (5) and 0.151 (5) Å, respectively (Fig. 1), indicating a boat conformation. Atom C3 deviates from the C1/C2/C4/C5/C6 plane by 0.658 (5) Å, indicating an envelope conformation. The dihedral angle between the C1/C6/C8/C17 plane and the C20–C25 benzene ring is 89.98 (11)°.

In the crystal structure, the molecules are connected *via*  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds (Table 1), forming chains along the  $a$  axis (Fig. 2).

## Experimental

Compound (I) was prepared by the reaction of 4-bromobenzaldehyde (1 mmol) with 3,3-dimethylcyclopentane-1,3-dione



**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

(1 mmol) and 2-naphthylamine (1 mmol) in ethanol (3 ml) at 351 K. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 95%; m.p. >573 K). Spectroscopic analysis:  $^1\text{H}$  NMR (DMSO- $d_6$ ,  $\delta$ , p.p.m.): 0.84 (3H, s, CH<sub>3</sub>), 1.04 (3H, s, CH<sub>3</sub>), 2.03 (1H, d,  $J$  = 16.4 Hz, CH<sub>2</sub>), 2.23 (1H, d,  $J$  = 16.4 Hz, CH<sub>2</sub>), 2.39 (1H, d,  $J$  = 16.8 Hz, CH<sub>2</sub>), 2.56 (1H, d,  $J$  = 16.8 Hz, CH<sub>2</sub>), 5.78 (1H, s, CH), 7.18 (2H, d,  $J$  = 8.4 Hz, ArH), 7.34–7.31 (4H, m, ArH), 7.42 (1H, t,  $J$  = 7.6 Hz, ArH), 7.82–7.79 (2H, m, ArH), 7.90 (1H, d,  $J$  = 8.4 Hz, ArH), 9.76 (1H, s, NH).

#### Crystal data

$\text{C}_{25}\text{H}_{22}\text{BrNO}$   
 $M_r = 432.35$   
 Triclinic,  $P\bar{1}$   
 $a = 7.296$  (4) Å  
 $b = 9.597$  (5) Å  
 $c = 15.304$  (8) Å  
 $\alpha = 94.038$  (7)°  
 $\beta = 93.465$  (8)°  
 $\gamma = 103.331$  (7)°

$V = 1036.9$  (9) Å<sup>3</sup>  
 $Z = 2$   
 $D_x = 1.385$  Mg m<sup>-3</sup>  
 Mo  $K\alpha$  radiation  
 $\mu = 2.00$  mm<sup>-1</sup>  
 $T = 298$  (2) K  
 Block, colourless  
 $0.32 \times 0.27 \times 0.09$  mm

#### Data collection

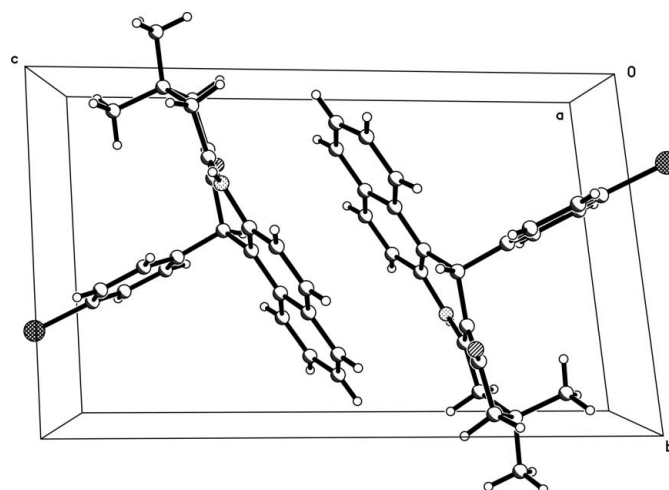
Bruker SMART CCD area-detector diffractometer  
 $\varphi$  and  $\omega$  scans  
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)  
 $T_{\min} = 0.567$ ,  $T_{\max} = 0.841$

5522 measured reflections  
 3346 independent reflections  
 2053 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.023$   
 $\theta_{\text{max}} = 25.0^\circ$

#### Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.044$   
 $wR(F^2) = 0.119$   
 $S = 1.01$   
 3346 reflections  
 253 parameters  
 H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0454P)^2 + 0.7039P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\text{max}} = 0.001$   
 $\Delta\rho_{\text{max}} = 0.60$  e Å<sup>-3</sup>  
 $\Delta\rho_{\text{min}} = -0.48$  e Å<sup>-3</sup>



**Figure 2**

A packing diagram for (I), projected along the  $a$  axis.

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N1-H1}\cdots\text{O1}^i$	0.86	1.99	2.840 (4)	172

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

All H atoms were positioned geometrically and treated as riding, with C–H distances in the range 0.93–0.98 Å, and with  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$  for methyl H atoms and  $1.2U_{\text{eq}}(\text{C})$  for others.

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.

The authors thank the National Natural Science Foundation of China (grant No. 20372057), the Natural Science Foundation of Jiangsu Province (grant No. BK2001142) and the Key Laboratory of Biotechnology for Medicinal Plants of Jiangsu Province (grant No. 01AXL 14) for financial support.

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