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10-Benzyl-7,8-dihydro-7,7-dimethyl-5-phenyl-5*H*-indeno[1,2-*b*]quinoline-9,11(6*H*,10*H*)-dione

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Key indicators

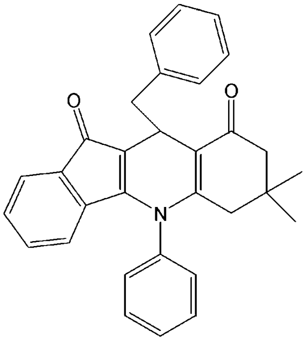
Single-crystal X-ray study
T = 173 K
Mean σ(C–C) = 0.003 Å
R factor = 0.056
wR factor = 0.110
Data-to-parameter ratio = 13.4

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

In the molecule of the title compound, $C_{31}H_{27}NO_2$, the dihydropyridine and cyclohexene rings adopt flattened-boat and envelope conformations, respectively. The molecules are linked by intermolecular C—H···O hydrogen bonds, forming a chain structure.

Comment

Multicomponent reactions (MCRs) occupy an outstanding position in organic and medicinal chemistry for their high degree of atom economy, application in combinatorial chemistry and diversity-oriented synthesis (Ramón & Yus, 2005; Burke & Schreiber, 2004; Andreana *et al.*, 2004). It is well known that indenoquinoline derivatives show a diverse range of biological properties, such as antitumour agents, acetylcholonesterase inhibitors and potent new cytotoxic agents (Deady *et al.*, 1999, 2000; Rampa *et al.*, 2000; Yamato *et al.*, 1989). In this paper, we report the crystal structure of the title compound, (I).



(I)

In the molecule of compound (I) (Fig. 1), the bond lengths and angles are in normal ranges (Allen *et al.*, 1987).

An examination of the deviations from the least-squares planes through the individual rings shows that rings *A* (C7–C12), *B* (C19–C24) , *C* (C26–C31) and *D* (C1/C2/C6/C7/C12) are planar. Rings *E* (N1/C1–C5) and *F* (C4/C5/C13–C16) are, of course, not planar. Ring *E* adopts a flattened-boat conformation, with puckering parameters (Cremer & Pople, 1975) $\varphi_2 = 121.56\ (2)^\circ$, $\theta_2 = 73.81\ (2)^\circ$ and $Q_T = 0.154\ (2)$ Å, while the conformation of ring *F* is an envelope [$\varphi_2 = -110.34\ (2)^\circ$, $\theta_2 = 24.25\ (2)^\circ$ and $Q_T = 0.468\ (2)$ Å] with atom C15 at the flap position, 0.625 (3) Å from the mean plane through the other five atoms.

The crystal structure of (I) is stabilized by intermolecular C—H···O hydrogen bonds (Table 1), resulting in the formation of a chain structure (Fig. 2).

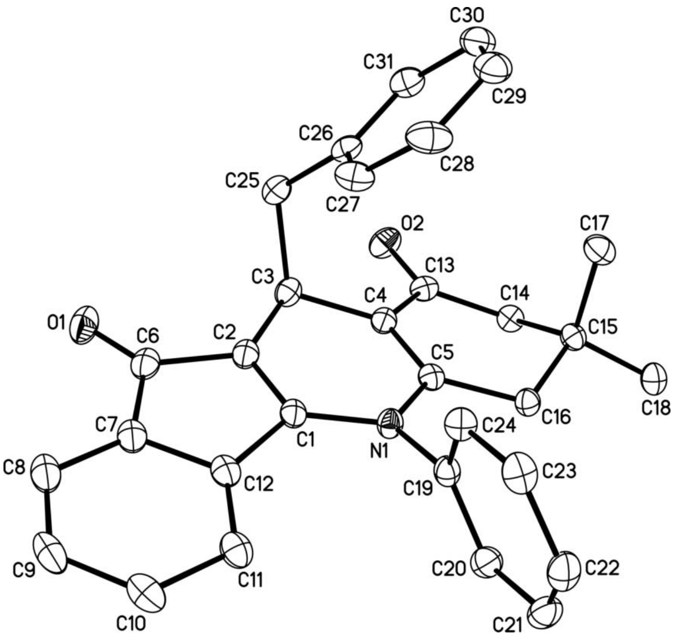


Figure 1
A drawing of the title molecular structure, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms have been omitted for clarity.

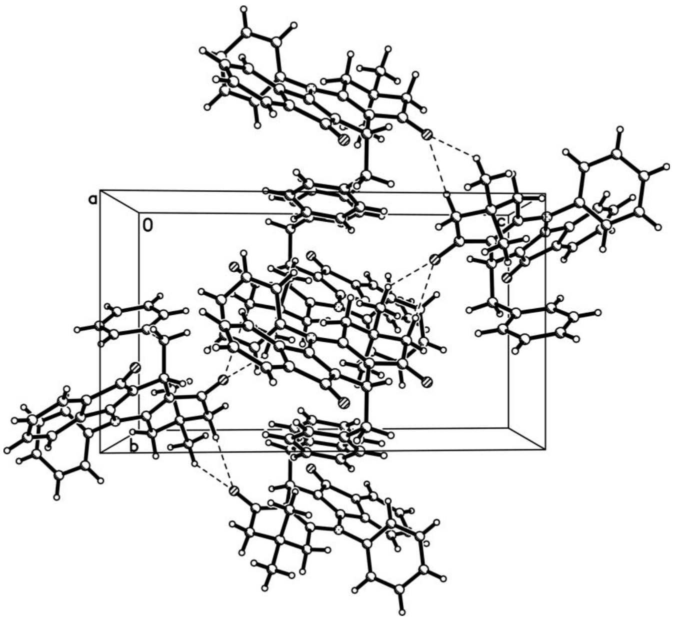


Figure 2
A packing diagram of (I). Hydrogen bonds are shown as dashed lines.

Experimental

The title compound was prepared by the reaction of 2-phenylacetaldehyde (120 mg, 1.0 mmol), 3-(phenylamino)-5,5-dimethylcyclohex-2-enone (220 mg, 1.0 mmol) and 1,3-indanedione (150 mg, 1.0 mmol) in a mixed solvent of glycol (0.5 ml) and acetic acid (1.0 ml) under microwave irradiation. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 380 mg, 85%; m.p. 480–482 K). Spectroscopic analysis: IR (KBr, cm^{-1}): 1686 (CO), 1637 (CO).

Crystal data

$C_{31}H_{27}NO_2$
$M_r = 445.54$
Monoclinic, $P2_1/n$
$a = 14.783$ (2) Å
$b = 9.4408$ (12) Å
$c = 16.345$ (2) Å
$\beta = 96.878$ (3)°
$V = 2264.6$ (5) Å^3
$Z = 4$
$D_x = 1.307$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.08$ mm^{-1}
$T = 173$ (2) K
Block, red
0.79 × 0.32 × 0.14 mm

Data collection

Rigaku Mercury diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{\min} = 0.939$, $T_{\max} = 0.989$
21579 measured reflections
4144 independent reflections
3611 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.040$
$\theta_{\max} = 25.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.110$
$S = 1.18$
4144 reflections
310 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0325P)^2 + 0.9725P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} < 0.001$
$\Delta\rho_{\max} = 0.20$ e Å^{-3}
$\Delta\rho_{\min} = -0.18$ e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14B···O2$^{\rm i}$	0.99	2.40	3.337 (2)	157
C18—H18A···O2$^{\rm i}$	0.98	2.58	3.429 (2)	145

Symmetry code: (i) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{3}{2}$.

H atoms were positioned geometrically, with C—H = 0.95, 0.98, 0.99 and 1.00 Å for aromatic, methyl, methylene and methine H, respectively, and were constrained to ride on their parent atoms, with $U_{\rm iso}({\rm H}) = xU_{\rm eq}({\rm C})$, where $x = 1.5$ for methyl H and $x = 1.2$ for all other H.

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*.

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