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5-Cyclopropyl-7,7-dimethyl-10-(4-nitrophenyl)-7,8-dihydro-5*H*-indeno[1,2-*b*]quinoline-9,11(6*H*,10*H*)-dione

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The title compound, $C_{27}H_{24}N_2O_4$, has been synthesized by the reaction of 4-nitrobenzaldehyde, 3-(cyclopropylamino)-5,5-dimethylcyclohex-2-enone and 1,3-indanedione in a mixed solvent of ethylene glycol and acetic acid under microwave irradiation. The dihydropyridine ring adopts a boat conformation. The molecules are linked by intermolecular C—H···O hydrogen bonds, forming a three-dimensional network structure.

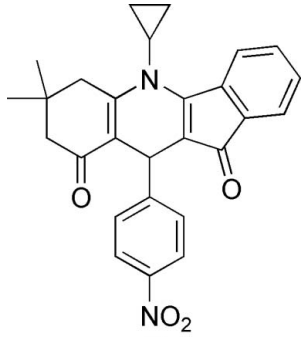
Key indicators

Single-crystal X-ray study
T = 153 K
Mean σ(C–C) = 0.003 Å
R factor = 0.062
wR factor = 0.124
Data-to-parameter ratio = 13.2

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

Comment

1,4-Dihydropyridines (1,4-DHPs) are well known for their pharmacological profiles as calcium channel modulators (Stout & Meyers, 1982). With a 1,4-DHP parent nucleus, indenoquinoline belongs to a class of compounds that are special not only because of their interesting chemical and physical properties, but also because of their immense utility in the pharmaceutical industry. The discovery that indenoquinoline is a potent cytotoxic and antitumor agent has attracted the attention of organic chemists (Yamato *et al.*, 1989; Deady *et al.*, 2000; Chen *et al.*, 2002). It is well established that chemical modifications of the indenoquinoline skeleton may bring remarkable changes in biological activity (Deady *et al.*, 1999). In this paper, we report the crystal structure of such a compound, (I).



(I)

In (I), the dihydropyridine ring adopts a boat conformation, with atoms C3 and N1 deviating from the C1/C2/C4/C5 plane by 0.281 (2) and 0.1761 (18) Å, respectively (Fig. 1). The cyclohexene ring adopts a twist-boat conformation: atoms C7 and C8 deviate from the C1/C2/C6/C9 plane by 0.112 (3) and −0.554 (2) Å, respectively. The dihedral angle between the C1/C2/C4/C5 plane and the C17–C22 benzene ring is 73.29 (12)°. The crystal structure is stabilized by intermolecular C—H···O hydrogen bonds (Table 1), resulting in the formation of a three-dimensional network.

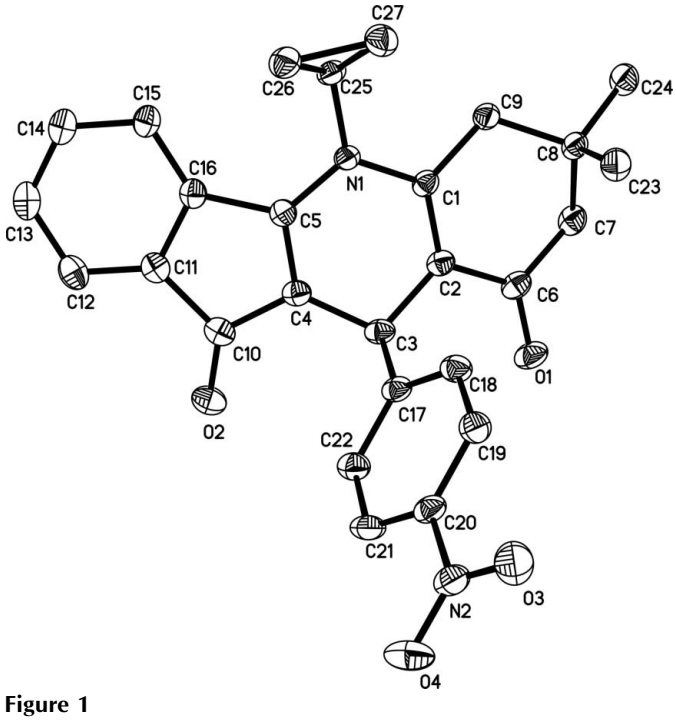


Figure 1
The molecular structure of (I), showing the atom-numbering scheme and 30% probability displacement ellipsoids. H atoms have been omitted.

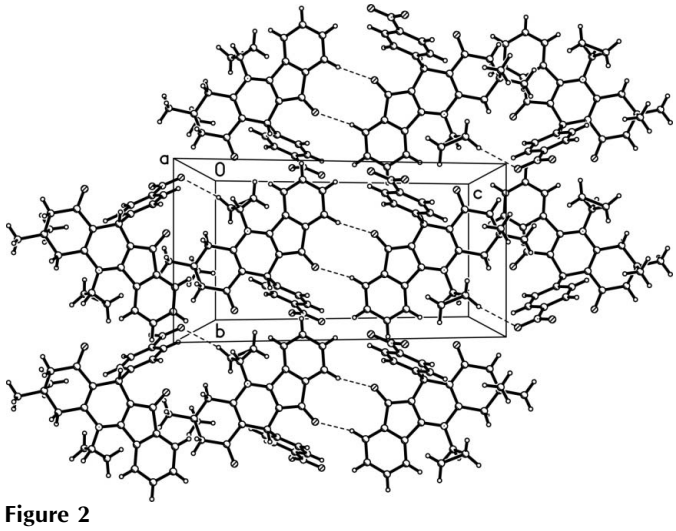


Figure 2
The packing of (I), projected along the *a* axis. Dashed lines indicate hydrogen bonds.

Experimental

The title compound, (I), was prepared by the reaction of 4-nitrobenzaldehyde (1 mmol), 3-(cyclopropylamino)-5,5-dimethylcyclohex-2-enone (1 mmol) and 1,3-indanedione (1 mmol) in a mixed solvent of ethylene glycol (0.5 ml) and acetic acid (1.0 ml) under microwave irradiation for 4 min at 200 W power and 393 K (Emrys Creator microwave oven from Personal Chemistry, Uppsala, Sweden). Upon completion, monitored by thin-layer chromatography, the reaction mixture was cooled to room temperature and then poured into cold water. The solid product was filtered, washed with water and EtOH (95%), and subsequently dried and recrystallized from EtOH (95%) to give the pure product. Single crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation of a 95% aqueous ethanol solution (yield 94%; m.p. 541–543 K).

Crystal data

$C_{27}H_{24}N_2O_4$
M_r = 440.48
Monoclinic, $C2/c$
a = 28.768 (5) Å
b = 8.9966 (12) Å
c = 17.703 (3) Å
β = 108.727 (4)°
V = 4339.2 (12) Å^3
Z = 8
D_x = 1.349 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 153 (2) K
Block, red
0.64 × 0.26 × 0.15 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.743, T_{max} = 0.986
20588 measured reflections
3964 independent reflections
3408 reflections with $I > 2\sigma(I)$
R_{int} = 0.043
θ_{max} = 25.4°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.124
S = 1.20
3964 reflections
301 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.038P)^2 + 3.838P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C27—H27B···O4^{i}	0.99	2.53	3.496 (3)	164
C27—H27A···O3^{ii}	0.99	2.55	3.262 (3)	129
C12—H12···O2^{iii}	0.95	2.55	3.298 (3)	136

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

All H atoms were positioned geometrically and treated as riding, with C—H distances of 0.95–1.00 Å and with U_{iso}(H) = 1.5U_{eq}(C) for methyl H atoms and 1.2U_{eq}(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*.

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