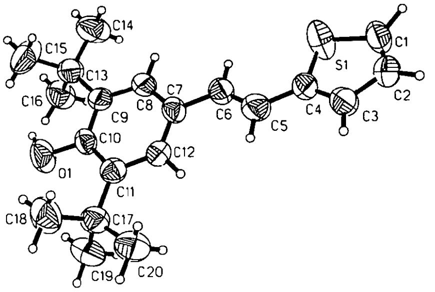

Fig. 1. Structure of the title compound. The ellipsoids are shown at 50% probability level.

Plus. The calculations of geometrical data and crystal packing were computed using the program *PARST* (Nardelli, 1983). All computations were carried out on a VAX 3100 work station. Table 1 gives the atomic coordinates and equivalent isotropic thermal parameters* and Table 2 lists bond distances and angles. Fig. 1 shows a perspective view of the molecule with the adopted numbering scheme and Fig. 2 gives a view of the unit cell along the *c* axis.

Related literature. The 2,6-di-*tert*-butylphenol derivatives appear to represent a new class of non-steroidal anti-inflammatory drugs with antioxidant properties (Ikuta, Shirota, Kobayashi, Yamagishi, Yamada, Yamatsu & Katayama, 1987). The title compound is one of a series of related compounds prepared by Lazer, Wong, Possanza, Graham & Farina (1989) that have anti-inflammatory activity. In all essential details the geometry of the molecule in terms of bond lengths and angles shows normal values (Tenon, Ebby, Voglozin, Degny, N'Guessan, Baldy, Pierrot & Bodot, 1989; Bernstein, 1975; Tirado-Rives, Fronczek & Gandour, 1985).

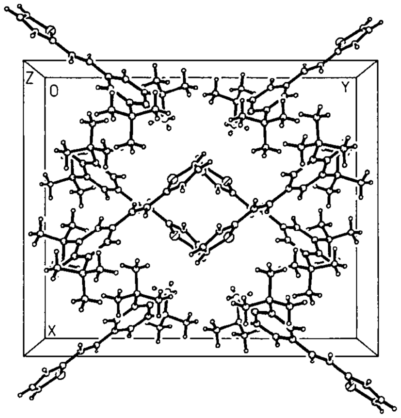

Fig. 2. The unit cell viewed down the *c* axis.

The assistance of Miss Madhavi Bhogaraju is gratefully acknowledged.

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* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54789 (9 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Structure of (3*R*,6*S*,12b*R*)-6-Cyanomethyl-3-ethyl-2-oxo-1,2,3,4,7,7a,12a,12b-octahydro-6*H*-indolo[2,3-*a*]quinolizine

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Abstract. $C_{19}H_{21}N_3O$, $M_r = 307.40$, monoclinic, $P2_1/c$, $a = 12.200\,(7)$, $b = 16.795\,(2)$, $c = 16.655\,(1)$ Å, $\beta = 104.18\,(3)°$, $V = 3308\,(3)$ Å^3, $Z = 8$, $D_x = 1.234$ g cm^{-3}, $\lambda(\text{Mo } K\alpha) = 0.71073$ Å, $\mu = 0.73$ cm^{-1}, $F(000) = 1312$, $T = 296$ K, final $R = 0.051$ for 2227 independent observed reflections. The two

Table 1. *Data-collection and refinement summary*

Data collection[i,ii]	
Mode	ω–2θ
Scan rate (° min^{-1})	1.56–5.49
θ range (°)	0–23
Range of *hkl*	$-13 \le h \le 12$, $0 \le k \le 18$, $0 \le l \le 18$
Total reflections measured	4980
Unique reflections	4590
$R_{\rm int}$	0.035
Approximate crystal dimensions (mm)	0.30 × 0.45 × 0.45
Structure determination and refinement[iii]	
Reflections used [$I > 3\sigma(I)$]	2227
No. of variables	417
R, wR	0.051, 0.048
Maximum, minimum density in final difference map (e Å^{-3})	0.16, −0.19
S	2.24

Notes: (i) Unit-cell parameters by least-squares refinement of the setting angles of 16 reflections with $10 < \theta < 15°$. (ii) Enraf–Nonius CAD-4 diffractometer with graphite monochromator. One standard reflection measured every hour showed no significant variation. (iii) Function minimized was $\sum w(|F_o| - |F_c|)^2$, where $w^{-1} = \sigma^2(F_o) + 0.0002F_o^2$.

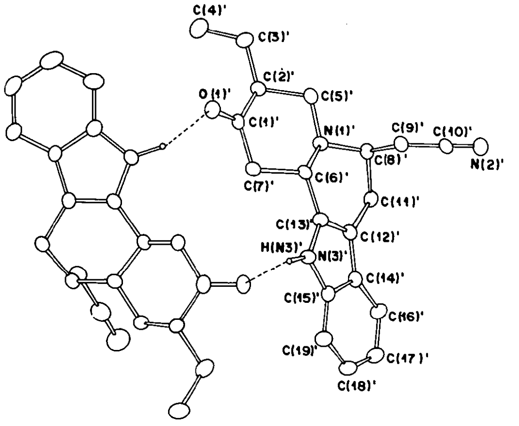

Fig. 1. Perspective view of the molecules showing the crystallographic atom labelling of one of the independent molecules and the hydrogen-bonding scheme.

independent enantiomeric molecules in the asymmetric unit are hydrogen bonded through N(3)···O(1′) [2.868 (4) Å] and N(3′)···O(1) [2.969 (4) Å]. The junction N(1)—C(6) is *trans* and the group CH_2CN is axial.

Experimental. Crystals were obtained from ethanol by slow evaporation at 293 K. Details of data collection and refinement parameters are summarized in Table 1. The structure was solved using standard direct methods and difference Fourier techniques. In the final cycles of least-squares refinement all non-H atoms were treated anisotropically. H atoms were included as fixed contributors, with overall isotropic temperature factors: for methyl H atoms $U = 0.077$ (2) Å^2, and for all others $U = 0.130$ (7) Å^2. Absorption corrections were not considered necessary. The maximum value of Δ/σ in the final refinement cycle was 0.09. Scattering factors for non-H atoms were taken from Cromer & Mann (1968) with corrections for anomalous dispersion from Cromer & Liberman (1970); for H atoms from Stewart, Davidson & Simpson (1965). Programs used: *SHELX76* (Sheldrick, 1976) and *ORTEP* (Johnson, 1965).

Table 2. *Final atomic coordinates and equivalent isotropic temperature factors* (Å^2)

$$B_{\rm eq} = (4/3)\sum_i\sum_j \beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$
N(1)	0.1138 (3)	0.5982 (2)	0.2042 (2)	3.6 (1)
N(2)	−0.1028 (4)	0.5796 (3)	−0.0145 (3)	8.0 (2)
N(3)	0.4133 (3)	0.5712 (2)	0.1945 (2)	3.7 (1)
O(1)	0.1328 (2)	0.3711 (2)	0.2680 (2)	5.3 (1)
C(1)	0.1327 (4)	0.4436 (3)	0.2731 (2)	4.1 (2)
C(2)	0.0294 (3)	0.4922 (2)	0.2737 (2)	3.9 (2)
C(3)	−0.0755 (4)	0.4407 (3)	0.2697 (2)	5.2 (2)
C(4)	−0.1719 (4)	0.4867 (3)	0.2920 (3)	7.0 (2)
C(5)	0.0119 (3)	0.5508 (2)	0.2010 (2)	4.2 (2)
C(6)	0.2099 (3)	0.5470 (2)	0.1974 (2)	3.4 (2)
C(7)	0.2363 (3)	0.4911 (2)	0.2738 (2)	3.7 (1)
C(8)	0.0959 (3)	0.6694 (2)	0.1515 (3)	4.1 (2)
C(9)	0.0801 (3)	0.6550 (2)	0.0578 (3)	4.7 (2)
C(10)	−0.0231 (5)	0.6122 (3)	0.0176 (3)	5.6 (2)
C(11)	0.1964 (3)	0.7260 (2)	0.1813 (2)	4.2 (2)
C(12)	0.3039 (4)	0.6800 (3)	0.1864 (2)	3.6 (2)
C(13)	0.3066 (3)	0.5998 (3)	0.1949 (2)	3.6 (2)
C(14)	0.4136 (4)	0.7051 (3)	0.1798 (2)	3.7 (2)
C(15)	0.4791 (4)	0.6360 (3)	0.1846 (2)	3.7 (2)
C(16)	0.4617 (4)	0.7787 (3)	0.1696 (2)	4.7 (2)
C(17)	0.5717 (5)	0.7806 (3)	0.1645 (3)	5.4 (2)
C(18)	0.6362 (4)	0.7114 (4)	0.1680 (3)	5.6 (2)
C(19)	0.5916 (4)	0.6377 (3)	0.1790 (2)	4.8 (2)
N(1′)	0.4048 (3)	0.2262 (2)	0.0480 (2)	3.3 (1)
N(2′)	0.4004 (3)	−0.0599 (2)	0.0429 (3)	7.6 (2)
N(3′)	0.1625 (3)	0.2519 (2)	0.1434 (2)	3.7 (1)
O(1′)	0.5241 (2)	0.4262 (2)	0.1688 (2)	5.0 (1)
C(1′)	0.4797 (4)	0.3757 (2)	0.1183 (3)	4.1 (2)
C(2′)	0.5387 (3)	0.3368 (2)	0.0585 (2)	3.9 (2)
C(3′)	0.6618 (4)	0.3623 (3)	0.0710 (3)	5.4 (2)
C(4′)	0.6766 (4)	0.4458 (3)	0.0393 (3)	6.5 (2)
C(5′)	0.5252 (3)	0.2458 (2)	0.0644 (2)	3.9 (2)
C(6′)	0.3563 (3)	0.2566 (2)	0.1146 (2)	3.2 (1)
C(7′)	0.3614 (3)	0.3476 (2)	0.1128 (2)	4.0 (2)
C(8′)	0.3803 (3)	0.1427 (2)	0.0254 (2)	3.5 (2)
C(9′)	0.4221 (3)	0.0845 (3)	0.0996 (2)	4.4 (2)
C(10′)	0.4106 (4)	0.0021 (3)	0.0692 (3)	5.1 (2)
C(11′)	0.2529 (3)	0.1332 (2)	−0.0139 (2)	3.7 (1)
C(12′)	0.1900 (3)	0.1723 (2)	0.0420 (2)	3.2 (1)
C(13′)	0.2378 (3)	0.2269 (2)	0.0993 (2)	3.3 (2)
C(14′)	0.0758 (4)	0.1624 (2)	0.0470 (3)	3.5 (2)
C(15′)	0.0600 (4)	0.2134 (2)	0.1110 (3)	3.4 (2)
C(16′)	−0.0163 (4)	0.1171 (2)	0.0046 (3)	4.3 (2)
C(17′)	−0.1181 (4)	0.1235 (3)	0.0260 (3)	5.5 (2)
C(18′)	−0.1308 (4)	0.1749 (3)	0.0891 (3)	5.3 (2)
C(19′)	−0.0423 (4)	0.2202 (3)	0.1333 (3)	4.6 (2)

Atomic coordinates for non-H atoms are given in Table 2,* interatomic distances and angles are given in Table 3. Fig. 1 is a projection of the title compound showing the atom-numbering scheme for one of the independent molecules.

Related literature. The title compound is a key intermediate in the reaction pathway for the synthesis of sarpagines (Braga, 1989). The knowledge of its

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* Lists of H-atom positions, anisotropic thermal parameters and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54710 (25 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: LI0101]

Table 3. *Interatomic distances* (Å) *and angles* (°)

N(1)—C(5)	1.466 (5)	N(1′)—C(5′)	1.464 (5)
N(1)—C(6)	1.481 (5)	N(1′)—C(6′)	1.471 (5)
N(1)—C(8)	1.468 (5)	N(1′)—C(8′)	1.464 (5)
N(2)—C(10)	1.130 (7)	N(2′)—C(10′)	1.125 (7)
N(3)—C(13)	1.389 (6)	N(3′)—C(13′)	1.375 (5)
N(3)—C(15)	1.386 (6)	N(3′)—C(15′)	1.394 (5)
O(1)—C(1)	1.221 (6)	O(1′)—C(1′)	1.224 (5)
C(1)—C(2)	1.504 (6)	C(1′)—C(2′)	1.513 (6)
C(1)—C(7)	1.492 (6)	C(1′)—C(7′)	1.500 (6)
C(2)—C(3)	1.533 (6)	C(2′)—C(3′)	1.526 (6)
C(2)—C(5)	1.534 (5)	C(2′)—C(5′)	1.543 (6)
C(3)—C(4)	1.527 (7)	C(3′)—C(4′)	1.525 (6)
C(6)—C(7)	1.550 (5)	C(6′)—C(7′)	1.530 (5)
C(6)—C(13)	1.485 (6)	C(6′)—C(13′)	1.491 (6)
C(8)—C(9)	1.544 (6)	C(8′)—C(9′)	1.560 (5)
C(8)—C(11)	1.535 (6)	C(8′)—C(11′)	1.540 (6)
C(9)—C(10)	1.462 (7)	C(9′)—C(10′)	1.468 (7)
C(11)—C(12)	1.506 (6)	C(11′)—C(12′)	1.496 (6)
C(12)—C(13)	1.354 (6)	C(12′)—C(13′)	1.349 (6)
C(12)—C(14)	1.433 (7)	C(12′)—C(14′)	1.426 (6)
C(14)—C(15)	1.400 (7)	C(14′)—C(15′)	1.417 (6)
C(14)—C(16)	1.396 (7)	C(14′)—C(16′)	1.397 (6)
C(15)—C(19)	1.399 (7)	C(15′)—C(19′)	1.391 (7)
C(16)—C(17)	1.366 (8)	C(16′)—C(17′)	1.378 (7)
C(17)—C(18)	1.397 (8)	C(17′)—C(18′)	1.398 (7)
C(18)—C(19)	1.382 (8)	C(18′)—C(19′)	1.377 (7)
C(5)—N(1)—C(6)	111.2 (3)	C(5′)—N(1′)—C(6′)	110.6 (3)
C(5)—N(1)—C(8)	114.8 (3)	C(5′)—N(1′)—C(8′)	113.3 (3)
C(6)—N(1)—C(8)	115.6 (3)	C(6′)—N(1′)—C(8′)	115.6 (3)
C(13)—N(3)—C(15)	107.4 (3)	C(13′)—N(3′)—C(15′)	107.8 (3)
O(1)—C(1)—C(2)	123.9 (4)	O(1′)—C(1′)—C(2′)	123.4 (4)
O(1)—C(1)—C(7)	121.2 (4)	O(1′)—C(1′)—C(7′)	121.2 (4)
C(2)—C(1)—C(7)	114.8 (4)	C(2′)—C(1′)—C(7′)	115.5 (3)
C(1)—C(2)—C(3)	112.7 (3)	C(1′)—C(2′)—C(3′)	113.6 (3)
C(1)—C(2)—C(5)	107.3 (3)	C(1′)—C(2′)—C(5′)	108.1 (3)
C(3)—C(2)—C(5)	112.0 (3)	C(3′)—C(2′)—C(5′)	112.7 (3)
C(2)—C(3)—C(4)	112.9 (4)	C(2′)—C(3′)—C(4′)	114.0 (4)
N(1)—C(5)—C(2)	111.5 (3)	N(1′)—C(5′)—C(2′)	109.2 (3)
N(1)—C(6)—C(7)	107.3 (3)	N(1′)—C(6′)—C(7′)	107.8 (3)
N(1)—C(6)—C(13)	107.7 (3)	N(1′)—C(6′)—C(13′)	107.9 (3)
C(7)—C(6)—C(13)	112.2 (3)	C(7′)—C(6′)—C(13′)	111.9 (3)
C(1)—C(7)—C(6)	108.2 (3)	C(1′)—C(7′)—C(6′)	110.9 (3)
N(1)—C(8)—C(9)	116.1 (3)	N(1′)—C(8′)—C(9′)	113.0 (3)
N(1)—C(8)—C(11)	108.7 (3)	N(1′)—C(8′)—C(11′)	109.3 (3)
C(9)—C(8)—C(11)	108.4 (3)	C(9′)—C(8′)—C(11′)	111.8 (3)
C(8)—C(9)—C(10)	114.8 (4)	C(8′)—C(9′)—C(10′)	109.4 (3)
N(2)—C(10)—C(9)	179.0 (6)	N(2′)—C(10′)—C(9′)	177.3 (5)
C(8)—C(11)—C(12)	108.4 (3)	C(8′)—C(11′)—C(12′)	108.0 (3)
C(11)—C(12)—C(13)	121.0 (4)	C(11′)—C(12′)—C(13′)	122.7 (4)
C(11)—C(12)—C(14)	131.4 (4)	C(11′)—C(12′)—C(14′)	130.0 (4)
C(13)—C(12)—C(14)	107.5 (4)	C(13′)—C(12′)—C(14′)	107.3 (4)
N(3)—C(13)—C(6)	123.1 (4)	N(3′)—C(13′)—C(6′)	123.6 (3)
N(3)—C(13)—C(12)	110.0 (4)	N(3′)—C(13′)—C(12′)	110.9 (3)
C(6)—C(13)—C(12)	126.7 (4)	C(6′)—C(13′)—C(12′)	125.6 (4)
C(12)—C(14)—C(15)	106.4 (4)	C(12′)—C(14′)—C(15′)	106.8 (4)
C(12)—C(14)—C(16)	134.3 (4)	C(12′)—C(14′)—C(16′)	135.3 (4)
C(15)—C(14)—C(16)	119.3 (4)	C(15′)—C(14′)—C(16′)	118.0 (4)
N(3)—C(15)—C(14)	108.6 (4)	N(3′)—C(15′)—C(14′)	107.3 (3)
N(3)—C(15)—C(19)	129.1 (4)	N(3′)—C(15′)—C(19′)	129.6 (4)
C(14)—C(15)—C(19)	122.3 (4)	C(14′)—C(15′)—C(19′)	123.1 (4)
C(14)—C(16)—C(17)	118.5 (4)	C(14′)—C(16′)—C(17′)	119.4 (4)
C(16)—C(17)—C(18)	122.0 (5)	C(16′)—C(17′)—C(18′)	121.0 (5)
C(17)—C(18)—C(19)	121.0 (5)	C(17′)—C(18′)—C(19′)	121.8 (5)
C(15)—C(19)—C(18)	116.9 (4)	C(15′)—C(19′)—C(18′)	116.7 (4)

molecular conformation may help in the prediction of the steric course of subsequent reactions. The two independent molecules are approximately related by an inversion centre, the main difference being the relative conformation of the nitrile and methyl groups. Superposition of the ring core of the two molecules gives a root-mean-square deviation between equivalent atoms of 0.11 Å (Kabsch, 1976).

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Structure of Di-*O*-methylscandenin: a Complex 4-Hydroxy-3-phenylcoumarin Derivative

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Abstract. 4,5-Dimethoxy-3-(4-methoxyphenyl)-8,8-dimethyl-6-(3-methyl-2-butenyl)-2*H*,8*H*-benzo[1,2-*b*:3,4-*b*′]dipyran-2-one, $C_{28}H_{30}O_6$, $M_r = 462.54$, monoclinic, $P2_1/c$, $a = 11.728$ (3), $b = 8.956$ (3), $c = 24.262$ (8) Å, $\beta = 103.98$ (1)°, $V = 2473$ (1) Å^3, $Z = 4$, D_m(flotation) = 1.239 (5), $D_x = 1.242$ g cm^{-3}, Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å, $\mu = 0.809$ cm^{-1}, $F(000) = 984$, $T = 294$ K, final $R = 0.079$ for 1197 reflections [$I \geq 3\sigma(I)$]. The coumarin ring system is nearly planar. The phenyl ring attached to this system is also planar and the dihedral angle between the phenyl and coumarin rings is 47.5 (3)°. The mean plane of the isoprenyl side chain makes an angle of 79.5 (4)° with the mean plane of the coumarin ring system. The angularly fused pyran ring is in a half-chair conformation.

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