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 (6)
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)

Table 3 (*cont.*)

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)-$2H,8H$-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.

Table 1. *Fractional coordinates and equivalent isotropic thermal parameters* ($Å^2 \times 10^3$) *with e.s.d.'s in parentheses*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
O1	0.801 (1)	0.610 (1)	0.2819 (3)	43 (3)
O2	0.964 (1)	0.517 (1)	0.3335 (3)	53 (3)
O3	1.378 (1)	0.883 (1)	0.4938 (4)	70 (4)
O4	0.888 (1)	1.026 (1)	0.3482 (3)	56 (3)
O5	0.692 (1)	1.132 (1)	0.2711 (3)	47 (3)
O6	0.433 (1)	0.770 (1)	0.1703 (3)	54 (3)
C1	0.938 (1)	0.779 (1)	0.3402 (4)	32 (3)
C2	0.862 (1)	0.890 (1)	0.3240 (5)	46 (4)
C3	0.751 (1)	0.870 (1)	0.2814 (4)	41 (4)
C4	0.671 (1)	0.984 (1)	0.2570 (4)	30 (4)
C5	0.564 (1)	0.950 (1)	0.2190 (4)	35 (3)
C6	0.542 (1)	0.798 (1)	0.2042 (4)	38 (4)
C7	0.420 (1)	0.637 (1)	0.1344 (5)	45 (4)
C8	0.488 (1)	0.511 (1)	0.1674 (5)	54 (5)
C9	0.582 (1)	0.533 (1)	0.2087 (5)	52 (5)
C10	0.622 (1)	0.685 (1)	0.2247 (4)	39 (4)
C11	0.726 (1)	0.727 (1)	0.2632 (4)	41 (4)
C12	0.910 (1)	0.630 (1)	0.3205 (4)	34 (3)
C13	1.055 (1)	0.800 (1)	0.3814 (4)	40 (4)
C14	1.129 (1)	0.913 (1)	0.3743 (4)	48 (4)
C15	1.237 (1)	0.939 (1)	0.4112 (5)	61 (5)
C16	1.272 (1)	0.850 (1)	0.4592 (4)	47 (4)
C17	1.203 (1)	0.737 (1)	0.4689 (5)	49 (4)
C18	1.094 (1)	0.713 (1)	0.4302 (4)	45 (4)
C19	1.425 (1)	0.788 (1)	0.5400 (6)	87 (6)
C20	0.475 (1)	1.067 (1)	0.1951 (5)	49 (5)
C21	0.480 (1)	1.111 (1)	0.1372 (5)	47 (4)
C22	0.395 (1)	1.121 (2)	0.0910 (6)	68 (6)
C23	0.274 (1)	1.078 (2)	0.0891 (6)	97 (8)
C24	0.414 (1)	1.170 (2)	0.0348 (6)	117 (10)
C25	0.464 (1)	0.670 (1)	0.0832 (5)	63 (5)
C26	0.291 (1)	0.602 (1)	0.1220 (6)	64 (5)
C27	0.780 (1)	1.196 (1)	0.2485 (6)	74 (6)
C28	0.821 (1)	1.058 (2)	0.3908 (8)	119 (10)

Experimental. Crystals were grown from ethanol solution as needles. Crystal data were measured on a crystal of dimensions $0.30 \times 0.25 \times 0.45$ mm. The unit-cell parameters and their e.s.d.'s were derived from 25 reflections with $25 < 2\theta < 40°$. Intensity data collected on an Enraf–Nonius CAD-4 diffractometer using monochromated Mo $K\alpha$ radiation, corrected for Lp; absorption ignored, scan width $(0.60 + 0.35\tan\theta)°$. Data collection with $3 < 2\theta < 55°$, $0 < h < 14$, $0 < k < 10$, $-34 < l < 34$; ω–2θ scan mode. Two standard reflections ($21\bar{9}$, $12\bar{9}$) measured every hour varied in intensity by $\leq 2\%$ during data collection. 3972 reflections measured of which 3664 were unique; 1197 with $I \geq 3\sigma(I)$ used in structural solution and refinement. Structure solved by direct methods with *SHELXTL-Plus* (Sheldrick, 1990); non-H atoms refined anisotropically; positions of H atoms calculated (C—H = 0.96 Å). H atoms assigned isotropic thermal parameters $U(H) = 1.2U_{eq}(C)$, and allowed to ride on parent C atoms. Final agreement factors were $R = 0.079$, $wR = 0.087$ [$w^{-1} = \sigma^2(F) + 0.0073F^2$] for 307 variables and 1197 observations, $S = 1.07$. Weak intensity data resulting from poor crystal quality lead to the rather poor ratio of observations to the number of parameters. Maximum (Δ/σ) in the final refinement cycle was 0.012. The final difference Fourier map showed no peaks higher than 0.37 e Å^{-3}. Atomic scattering factors as in

Table 2. *Bond lengths* (Å) *and bond angles* (°) *with e.s.d.'s in parentheses*

O1—C11	1.37 (1)	O1—C12	1.40 (1)
O2—C12	1.20 (1)	O3—C16	1.35 (1)
O3—C19	1.41 (1)	O4—C2	1.35 (1)
O4—C28	1.47 (2)	O5—C4	1.37 (1)
O5—C27	1.40 (1)	O6—C6	1.37 (1)
O6—C7	1.46 (1)	C1—C2	1.32 (1)
C1—C12	1.42 (1)	C1—C13	1.51 (1)
C2—C3	1.45 (1)	C3—C4	1.41 (4)
C3—C11	1.36 (1)	C4—C5	1.40 (1)
C5—C6	1.41 (1)	C5—C20	1.50 (1)
C6—C10	1.38 (1)	C7—C8	1.50 (1)
C7—C25	1.48 (1)	C7—C26	1.51 (1)
C8—C9	1.31 (1)	C9—C10	1.46 (1)
C10—C11	1.40 (1)	C13—C14	1.37 (1)
C13—C18	1.40 (1)	C14—C15	1.38 (1)
C15—C16	1.40 (1)	C16—C17	1.35 (1)
C17—C18	1.40 (1)	C20—C21	1.47 (1)
C21—C22	1.31 (1)	C22—C23	1.45 (2)
C22—C24	1.50 (2)		

C12—C1—C13	115.8 (9)	C2—C1—C12	121.1 (10)
C2—C1—C13	123.3 (9)	O4—C2—C1	118.5 (9)
C1—C2—C3	122.7 (9)	O4—C2—C3	118.8 (9)
C2—C3—C11	115.2 (9)	C2—C3—C4	126.8 (9)
C4—C3—C11	118.1 (9)	O5—C4—C3	121.8 (9)
C3—C4—C5	121.0 (9)	O5—C4—C5	117.0 (8)
C4—C5—C20	121.7 (9)	C4—C5—C6	117.5 (9)
C6—C5—C20	120.9 (9)	O6—C6—C5	114.6 (9)
C5—C6—C10	122.8 (9)	O6—C6—C10	122.6 (9)
O6—C7—C26	103.9 (9)	O6—C7—C25	109.4 (9)
O6—C7—C8	109.3 (9)	C25—C7—C26	114.4 (10)
C8—C7—C26	109.0 (10)	C8—C7—C25	110.5 (10)
C7—C8—C9	122.2 (11)	C8—C9—C10	120.1 (11)
C6—C10—C9	115.7 (10)	C9—C10—C11	127.1 (10)
C6—C10—C11	116.8 (9)	C3—C11—C10	123.6 (10)
O1—C11—C10	113.5 (9)	O1—C11—C3	122.8 (9)
O2—C12—C1	129.4 (9)	O1—C12—C1	116.4 (8)
O1—C12—O2	114.2 (8)	C1—C13—C18	123.4 (10)
C1—C13—C14	120.7 (9)	C14—C13—C18	115.8 (10)
C13—C14—C15	123.3 (11)	C14—C15—C16	119.2 (11)
O3—C16—C15	116.0 (11)	C15—C16—C17	120.2 (11)
O3—C16—C17	123.8 (11)	C16—C17—C18	119.1 (10)
C13—C18—C17	122.3 (10)	C5—C20—C21	111.9 (9)
C20—C21—C22	129.9 (11)	C21—C22—C24	123.3 (13)
C21—C22—C23	122.8 (13)	C23—C22—C24	113.8 (12)
C16—O3—C19	119.2 (10)	C2—O4—C28	112.4 (10)
C4—O5—C27	113.7 (8)	C6—O6—C7	116.9 (8)
C11—O1—C12	121.7 (7)		

SHELXTL-Plus; geometrical data and crystal packing computed by the program *PARST* (Nardelli, 1983).

Final atomic positions and equivalent isotropic temperature factors for the non-H atoms are given in Table 1.* Bond lengths and angles are listed in Table 2. A thermal-ellipsoid drawing (*SHELXTL-Plus*) of the molecule is shown in Fig. 1 and the molecular packing projected along the *ac* plane is in Fig. 2.

Related literature. Scandenin is an insecticide obtained from the root extract of *Derris scandens* (Falshaw, Harmer, Ollis, Wheeler, Lalitha & Subba Rao, 1969). It is characterized as a complex 4-hydroxy-3-phenylcoumarin (Johnson, Pelter & Stainton, 1966). In all essential details the geometry of the molecule, in terms of bond lengths and angles, shows
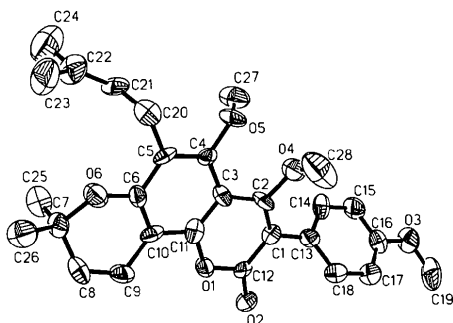
Fig. 1. The structure of di-O-methylscandenin. The ellipsoids are shown at the 50% probability level.
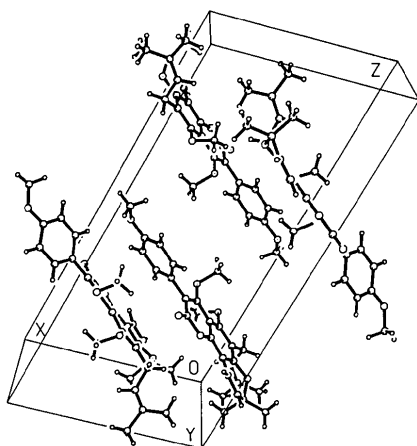
Fig. 2. The unit cell of di-O-methylscandenin looking down the b axis.

normal values (Murthy, Ramamurthy & Venkatesan, 1988; Schweizer & Dunitz, 1982; Wolska, Borowiak & Cisowski, 1991). The lengths of the C—O bonds in the pyran ring are similar to those in a variety of compounds incorporating the pyran ring (Gambardella, Mascarenhas & Santos, 1983; Jones, Kennard, Kirby & Martin, 1979; Ravikumar & Rajan, 1987).

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Structure of (E)-4-Hydroxyiminomethyl-1-(p-methoxyphenyl)imidazole

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Abstract. $C_{11}H_{11}N_3O_2$, $M_r = 217.2$, monoclinic, $P2_1/c$, $a = 9.009$ (5), $b = 7.882$ (2), $c = 15.072$ (7) Å, $\beta = 98.61$ (6)°, $V = 1058.3$ (8) Å^3, $Z = 4$, $D_x = 1.363$ Mg m^{-3}, $\lambda(Mo\ K\alpha) = 0.71069$ Å, $\mu = 0.091$ mm^{-1}, $F(000) = 456$, $T = 293$ (3) K, $R = 0.046$, $wR = 0.036$, $S = 1.99$, 4592 unique observed reflec-

tions with $F_o > 6\sigma(F_o)$. The structure consists of a monoclinic packing of a hydroxyimino oxime. The angle between the imidazole and phenyl groups is 43.3°. The mean deviations from the imidazole and phenyl planes are 0.0013 and 0.0035 Å, respectively. The molecules related by symmetry are linked by two hydrogen bonds between the hydroxy O atom and the unsubstituted N of the imidazole. C and N of the

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