screw axis. Thus three molecular stacks are formed about the three independent 3_1 axes of the unit cell, a packing diagram of which is shown in Fig. 2. Two of the stacks (from molecules *A* and *B*) have the same effective polarity with the O—H···O bonds directed along negative *c* (of the arbitrarily chosen $P3_1$ enantiomorph), whereas molecular stack *C* has the reverse orientation. The stack composed of molecules *A* is shown in Fig. 3. In 1-Me-DHI the packing is again dictated by hydrogen bonds and the molecules also associate in trigonal stacks with the hydrophilic groups at the center. In this case all 5-OH groups are linked to each other around a pure threefold axis and 6-OH···5-OH contacts link the molecules along the *c* glide. All molecules have the same polar orientation and the [001] and [00$\bar{1}$] faces are more readily chemically differentiated.

Bond lengths, angles and intermolecular contacts for 5-hydroxyindole are given in Table 2. No significant differences are found between the three independent molecules, with the exception of the exocyclic C—C—O angles which are influenced by the intermolecular hydrogen bonds. A deviation of more than 2.0° is found for molecule *B*, with C(6)—C(5)—O(5) greater and C(4)—C(5)—O(5) smaller than in molecules *A* or *C*. The average molecular dimensions for 5-hydroxyindole were not found to be significantly different from 1-Me-DHI or the mean values for 17 other indole structures in the Cambridge Structural Database (Allen, Kennard & Taylor, 1983).

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Structure of Ursolic Acid Ethanol Solvate

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Abstract. $C_{30}H_{48}O_3.C_2H_6O$, $M_r = 502.78$, orthorhombic, $P2_12_12_1$, $a = 7.199$ (1), $b = 12.157$ (2), $c = 33.888$ (2) Å, $V = 2966$ Å^3, $Z = 4$, $D_x = 1.13$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 5.3$ cm^{-1}, $F(000) = 1112$, $T = 298$ K, $R = 0.050$ for 1632 reflections with $I > 3\sigma(I)$. The rings adopt chair conformations. Crystal

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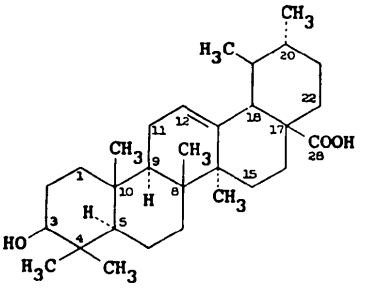
cohesion is ensured by a network of van der Waals contacts and hydrogen bonds with the ethanol adduct molecules.

Introduction. Ursolic acid (1) is a triterpene carboxylic acid often found in plants (Kowaleski, Kortus, Kedzia & Koniar, 1976). It inhibits tumor promotion in mouse skin in the same way as retinoic acid (Tokuda, Ohigashi, Koshimizu & Ito, 1986). Ursolic acid and its analogs may also inhibit the inflammation induced by tumor promoters (Hirota, Mori, Yoshida & Iriye, 1990); the results suggested that the C(3) hydroxyl group and the 4,4-dimethyl group were the essential factors for the inhibitory activity. The crystal structure of ursolic acid has been determined to establish its conformation and absolute configuration as part of a program correlating the biological activity and molecular structure of antitumor promoters (Allais, Simon, Bennini, Kaouadji, Chulia & Delage, 1991).



(1)

Experimental. Prismatic crystals of ursolic acid (Sigma) were obtained from a solution of ethanol by slow evaporation at room temperature; white crystal, dimensions 0.35 × 0.15 × 0.10 mm; unit-cell parameters from least-squares refinement of 25 reflections with $2 < \theta < 16°$; data collection on an Enraf–Nonius CAD-4 diffractometer, graphite-monochromated Cu $K\alpha$ radiation ($\lambda = 1.5418$ Å), $\omega/2\theta$ scan mode, ω-scan width $(1.0 + 0.150\tan\theta)°$, $2\theta_{max} = 120°$, 2638 unique reflections ($0 \le h \le 8$, $0 \le k \le 13$, $-4 \le l \le 38$); standard reflection $(02\bar{3})$ measured every hour showed no significant variations; Lorentz and polarization corrections, but no absorption correction; structure solved using *MULTAN*80 (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and Fourier methods; atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV); positions of all H atoms ideally calculated on the basis of stereochemical considerations and checked on a difference Fourier map calculated using the anisotropic non-H atoms; structure refined by full-matrix least squares with anisotropic temperature factors for non-H atoms and isotropic ones for H atoms; the final refinement including H atoms reduced R to 0.050 ($wR = 0.048$, $S = 1.03$) for 1632 reflections [$I \ge 3.0\sigma(I)$] and 316 parameters; $(\Delta/\sigma)_{max}$ in last cycle was 0.5; function minimized $\sum w(|F_o| - |F_c|)^2$, where $w = 1/\sigma(F_o)^2$; highest and lowest residuals in final difference Fourier map 0.13 (4) and 0.00 (4) e Å^{-3}; all crystallographic computations were performed on a MicroVAX II computer.

Table 1. *Fractional atomic coordinates and equivalent isotropic temperature factors* (Å^2) *for non-*H *atoms with e.s.d.'s in parentheses*

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

	x	y	z	B_{eq}
O(1)	0.7937 (7)	0.3065 (4)	0.8925 (1)	5.6 (1)
O(2)	0.6398 (7)	0.0151 (4)	0.5750 (2)	6.2 (1)
O(3)	0.9049 (8)	−0.0666 (4)	0.5841 (2)	6.5 (1)
C(1)	0.601 (1)	0.2841 (6)	0.7902 (2)	4.5 (2)
C(2)	0.600 (1)	0.2941 (6)	0.8349 (2)	4.8 (2)
C(3)	0.799 (1)	0.2900 (5)	0.8506 (2)	4.2 (2)
C(4)	0.8987 (9)	0.1822 (5)	0.8403 (2)	3.8 (1)
C(5)	0.8919 (8)	0.1712 (5)	0.7944 (2)	3.4 (1)
C(6)	0.9974 (9)	0.0732 (6)	0.7777 (2)	3.9 (2)
C(7)	1.0433 (9)	0.0937 (5)	0.7345 (2)	3.8 (1)
C(8)	0.8745 (9)	0.1186 (5)	0.7086 (2)	3.2 (1)
C(9)	0.7361 (9)	0.1985 (5)	0.7293 (2)	3.4 (1)
C(10)	0.6978 (8)	0.1800 (5)	0.7748 (2)	3.4 (1)
C(11)	0.560 (1)	0.2105 (6)	0.7043 (2)	4.9 (2)
C(12)	0.600 (1)	0.2152 (6)	0.6606 (2)	4.4 (2)
C(13)	0.7625 (9)	0.2008 (5)	0.6437 (2)	3.5 (1)
C(14)	0.9348 (9)	0.1746 (5)	0.6685 (2)	3.6 (1)
C(15)	1.0699 (9)	0.0993 (5)	0.6458 (2)	3.9 (1)
C(16)	1.093 (1)	0.1268 (5)	0.6023 (2)	4.5 (2)
C(17)	0.908 (1)	0.1305 (5)	0.5809 (2)	4.1 (2)
C(18)	0.7814 (9)	0.2181 (5)	0.5992 (2)	3.8 (1)
C(19)	0.836 (1)	0.3376 (6)	0.5886 (2)	4.6 (2)
C(20)	0.862 (1)	0.3530 (6)	0.5430 (2)	5.4 (2)
C(21)	0.995 (1)	0.2688 (6)	0.5270 (2)	6.0 (2)
C(22)	0.938 (1)	0.1518 (6)	0.5362 (2)	5.1 (2)
C(23)	1.107 (1)	0.1981 (6)	0.8525 (2)	5.2 (2)
C(24)	0.822 (1)	0.0837 (6)	0.8630 (2)	5.2 (2)
C(25)	0.776 (1)	0.0065 (6)	0.6998 (2)	4.8 (2)
C(26)	0.570 (1)	0.0804 (6)	0.7834 (2)	5.0 (2)
C(27)	1.041 (1)	0.2848 (5)	0.6759 (2)	4.0 (2)
C(28)	0.820 (1)	0.0164 (6)	0.5815 (2)	4.7 (2)
C(29)	0.692 (1)	0.4191 (6)	0.6038 (2)	6.6 (2)
C(30)	0.930 (2)	0.4677 (7)	0.5321 (3)	8.2 (3)

Discussion. The final atomic parameters of the non-H atoms and equivalent isotropic B_{eq}'s are given in Table 1. Bond lengths, angles and selected torsion angles are listed in Table 2.* A perspective view of ursolic acid showing the molecular structure with the numbering scheme is presented in Fig. 1.

Bond lengths and angles are very similar to those given in the literature for other triterpenes (Mahato & Nandy, 1990). The C_{sp^2}—C_{sp^2} bond distance in the molecule is 1.311 (9) Å and the C_{sp^3}—C_{sp^3} bond lengths range from 1.51 (1) to 1.582 (8) Å. The two C_{sp^3}—C_{sp^2} bond distances are 1.511 (9) and 1.532 (9) Å. The triterpene moiety consists of the five

* 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 54790 (36 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA0243]

Table 2. *Bond lengths* (Å), *bond angles* (°) *and selected torsion angles* (°) *for non-*H *atoms with e.s.d.'s in parentheses*

O(1)—C(3)	1.432 (8)	C(10)—C(26)	1.55 (1)
O(2)—C(28)	1.319 (9)	C(11)—C(12)	1.511 (9)
O(3)—C(28)	1.182 (9)	C(12)—C(13)	1.311 (9)
C(1)—C(2)	1.519 (9)	C(13)—C(14)	1.532 (9)
C(1)—C(10)	1.536 (9)	C(13)—C(18)	1.530 (9)
C(2)—C(3)	1.53 (1)	C(14)—C(15)	1.543 (9)
C(3)—C(4)	1.533 (9)	C(14)—C(27)	1.562 (9)
C(4)—C(5)	1.565 (8)	C(15)—C(16)	1.520 (9)
C(4)—C(23)	1.56 (1)	C(16)—C(17)	1.52 (1)
C(4)—C(24)	1.53 (1)	C(17)—C(18)	1.534 (9)
C(5)—C(6)	1.521 (9)	C(17)—C(22)	1.551 (9)
C(5)—C(10)	1.550 (8)	C(17)—C(28)	1.525 (9)
C(6)—C(7)	1.520 (9)	C(18)—C(19)	1.548 (9)
C(7)—C(8)	1.530 (9)	C(19)—C(20)	1.57 (1)
C(8)—C(9)	1.559 (9)	C(19)—C(29)	1.53 (1)
C(8)—C(14)	1.579 (8)	C(20)—C(21)	1.50 (1)
C(8)—C(25)	1.566 (9)	C(20)—C(30)	1.52 (1)
C(9)—C(10)	1.582 (8)	C(21)—C(22)	1.51 (1)
C(9)—C(11)	1.535 (9)		

C(2)—C(1)—C(10)	113.9 (5)	C(18)—C(19)—C(29)	110.9 (6)
C(1)—C(2)—C(3)	110.0 (6)	C(8)—C(9)—C(10)	117.5 (5)
O(1)—C(3)—C(2)	108.3 (5)	C(8)—C(9)—C(11)	109.8 (5)
O(1)—C(3)—C(4)	111.0 (5)	C(10)—C(9)—C(11)	114.1 (5)
C(2)—C(3)—C(4)	112.7 (5)	C(1)—C(10)—C(5)	108.7 (5)
C(3)—C(4)—C(5)	106.6 (5)	C(1)—C(10)—C(9)	107.0 (5)
C(3)—C(4)—C(23)	106.4 (5)	C(1)—C(10)—C(26)	108.0 (5)
C(3)—C(4)—C(24)	112.8 (5)	C(5)—C(10)—C(9)	105.6 (5)
C(5)—C(4)—C(23)	107.6 (5)	C(5)—C(10)—C(26)	113.8 (5)
C(5)—C(4)—C(24)	115.0 (5)	C(9)—C(10)—C(26)	113.4 (5)
C(23)—C(4)—C(24)	108.0 (5)	C(9)—C(11)—C(12)	112.6 (6)
C(4)—C(5)—C(6)	114.9 (5)	C(11)—C(12)—C(13)	126.6 (6)
C(4)—C(5)—C(10)	116.6 (5)	C(12)—C(13)—C(14)	120.6 (6)
C(6)—C(5)—C(10)	110.2 (5)	C(12)—C(13)—C(18)	119.5 (6)
C(5)—C(6)—C(7)	109.7 (5)	C(14)—C(13)—C(18)	119.8 (5)
C(6)—C(7)—C(8)	114.4 (5)	C(8)—C(14)—C(13)	109.8 (5)
C(7)—C(8)—C(9)	111.8 (5)	C(8)—C(14)—C(15)	110.3 (5)
C(7)—C(8)—C(14)	111.2 (5)	C(8)—C(14)—C(27)	111.5 (5)
C(7)—C(8)—C(25)	107.3 (5)	C(13)—C(14)—C(15)	111.1 (5)
C(9)—C(8)—C(14)	107.1 (5)	C(13)—C(14)—C(27)	107.9 (5)
C(9)—C(8)—C(25)	109.7 (5)	C(15)—C(14)—C(27)	106.3 (5)
C(14)—C(8)—C(25)	109.7 (5)	C(14)—C(15)—C(16)	115.1 (5)
C(16)—C(17)—C(18)	110.5 (5)	C(15)—C(16)—C(17)	111.9 (6)
C(16)—C(17)—C(22)	110.6 (6)	C(20)—C(19)—C(29)	109.6 (6)
C(16)—C(17)—C(28)	109.3 (5)	C(19)—C(20)—C(21)	110.5 (6)
C(18)—C(17)—C(22)	111.2 (5)	C(19)—C(20)—C(30)	112.9 (6)
C(18)—C(17)—C(28)	112.1 (6)	C(21)—C(20)—C(30)	109.3 (7)
C(22)—C(17)—C(28)	102.9 (5)	C(20)—C(21)—C(22)	113.3 (7)
C(13)—C(18)—C(17)	110.9 (5)	C(17)—C(22)—C(21)	113.3 (6)
C(13)—C(18)—C(19)	112.3 (5)	O(2)—C(28)—O(3)	120.6 (7)
C(17)—C(18)—C(19)	113.9 (5)	O(2)—C(28)—C(17)	114.7 (6)
C(18)—C(19)—C(20)	111.8 (5)	O(3)—C(28)—C(17)	124.4 (7)

C(10)—C(1)—C(2)—C(3)	56.6 (7)	C(11)—C(9)—C(10)—C(26)	55.2 (7)
C(2)—C(1)—C(10)—C(5)	−50.7 (7)	C(8)—C(9)—C(11)—C(12)	−39.1 (7)
C(2)—C(1)—C(10)—C(26)	73.1 (6)	C(9)—C(11)—C(12)—C(13)	6.1 (9)
C(1)—C(2)—C(3)—O(1)	176.4 (5)	C(11)—C(12)—C(13)—C(14)	1.0 (9)
C(1)—C(2)—C(3)—C(4)	−60.3 (7)	C(12)—C(13)—C(14)—C(8)	24.9 (7)
O(1)—C(3)—C(4)—C(5)	178.5 (4)	C(12)—C(13)—C(14)—C(27)	−96.7 (6)
C(2)—C(3)—C(4)—C(5)	56.8 (6)	C(18)—C(13)—C(14)—C(15)	−36.9 (7)
C(2)—C(3)—C(4)—C(23)	171.4 (5)	C(18)—C(13)—C(14)—C(27)	79.1 (6)
C(2)—C(3)—C(4)—C(24)	−70.3 (7)	C(14)—C(13)—C(18)—C(17)	44.0 (7)
C(3)—C(4)—C(5)—C(10)	−53.4 (6)	C(13)—C(14)—C(15)—C(16)	40.7 (7)
C(23)—C(4)—C(5)—C(10)	−167.2 (5)	C(27)—C(14)—C(15)—C(16)	−76.2 (6)
C(24)—C(4)—C(5)—C(10)	72.3 (7)	C(14)—C(15)—C(16)—C(17)	−54.3 (7)
C(10)—C(5)—C(6)—C(7)	67.1 (6)	C(15)—C(16)—C(17)—C(18)	59.8 (6)
C(4)—C(5)—C(10)—C(1)	50.5 (6)	C(16)—C(17)—C(18)—C(13)	−53.2 (6)
C(4)—C(5)—C(10)—C(26)	−69.8 (6)	C(22)—C(17)—C(18)—C(19)	−48.6 (7)
C(6)—C(5)—C(10)—C(9)	−61.5 (6)	C(28)—C(17)—C(18)—C(19)	−163.2 (5)
C(6)—C(5)—C(10)—C(26)	63.4 (6)	C(18)—C(17)—C(22)—C(21)	49.9 (8)
C(5)—C(6)—C(7)—C(8)	−56.1 (6)	C(28)—C(17)—C(22)—C(21)	170.2 (6)
C(6)—C(7)—C(8)—C(9)	42.3 (7)	C(22)—C(17)—C(28)—O(2)	−82.1 (6)
C(7)—C(8)—C(9)—C(10)	−40.9 (7)	C(22)—C(17)—C(28)—O(3)	91.2 (7)
C(14)—C(8)—C(9)—C(11)	64.4 (6)	C(17)—C(18)—C(19)—C(20)	50.7 (7)
C(25)—C(8)—C(9)—C(10)	77.9 (6)	C(17)—C(18)—C(19)—C(29)	173.3 (5)
C(25)—C(8)—C(9)—C(11)	−54.6 (6)	C(18)—C(19)—C(20)—C(21)	−52.9 (8)
C(9)—C(8)—C(14)—C(13)	−56.2 (6)	C(18)—C(19)—C(20)—C(30)	−175.7 (6)
C(25)—C(8)—C(14)—C(13)	62.8 (6)	C(29)—C(19)—C(20)—C(21)	−176.3 (6)
C(25)—C(8)—C(14)—C(15)	−59.9 (6)	C(19)—C(20)—C(21)—C(22)	55.6 (8)
C(25)—C(8)—C(14)—C(27)	−177.7 (5)	C(30)—C(20)—C(21)—C(22)	−179.5 (6)
C(8)—C(9)—C(10)—C(5)	49.8 (6)	C(20)—C(21)—C(22)—C(17)	−55.0 (8)
C(8)—C(9)—C(10)—C(26)	−75.4 (6)		

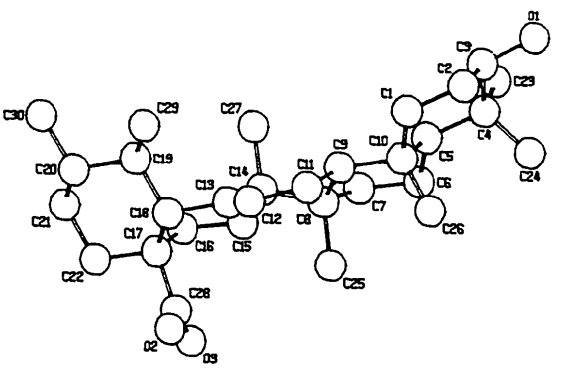


Fig. 1. A perspective view of the molecule with the atom-numbering scheme.

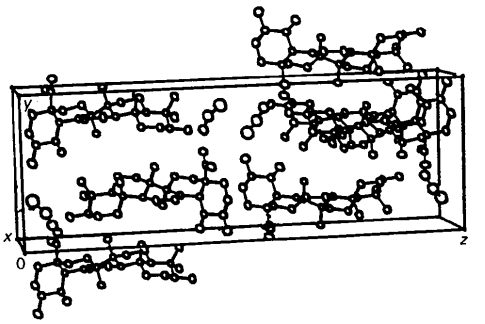


Fig. 2. Unit cell viewed along the *c* axis.

six-membered rings with chair conformations. The substituents are linked as follows: the carboxy group at C(17) and the methyl groups C(24), C(25), C(26), C(27) are axially substituted; OH and all other methyl groups [C(23), C(29), C(30)] are in equatorial positions. A perspective view of the crystal packing is shown in Fig. 2. Crystal cohesion is ensured by a three-dimensional network of van der Waals interactions and hydrogen bonds between the hydroxyl group of ursolic acid at C(3) and ethanol molecule [O(4)···O(1) = 2.609 (5) Å].

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