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Structure of Salbomycin, $C_{54}H_{88}O_{18}.2H_2O$

BY ERICH F. PAULUS AND LÁSZLÓ VERTESY

Hoechst AG, D-6230 Frankfurt 60, Federal Republic of Germany

AND GEORGE M. SHELDRICK

Institut für Anorganische Chemie der Universität, Tammannstrasse 4, D-3400 Göttingen, Federal Republic of Germany

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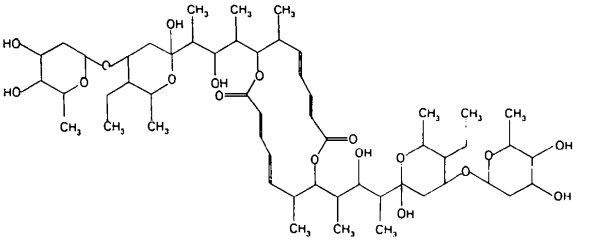
Abstract. Salbomycin, a new kind of antibiotic, has the systematic name 8,16-bis{3-[4-(4,5-dihydroxy-6-methyl-2-tetrahydropyranyloxy)-5-ethyl-2-hydroxy-6-methyl-2-tetrahydropyranyl]-2-hydroxy-1-methylbutyl}-7,15-dimethyl-1,9-dioxacyclohexadeca-3,5,11,13-tetraene-2,10-dione dihydrate. $M_r = 1061{\cdot}15$, monoclinic, $P2_1$, $a = 9{\cdot}770\ (2)$, $b = 10{\cdot}037\ (3)$, $c = 30{\cdot}890\ (5)$ Å, $\beta = 92{\cdot}58\ (2)°$, $U = 3026{\cdot}05$ Å^3, $Z = 2$, $D_m = 1{\cdot}17$ (flotation in CCl_4/*n*-heptane mixture), $D_x = 1{\cdot}165$ Mg m^{-3}, Cu $K\alpha$, $\lambda = 1{\cdot}54184$ Å, $\mu = 0{\cdot}672$ mm^{-1}, $F(000) = 1152$, $T = 140$ K, $R_2 = 0{\cdot}053$ for 3660 unique diffractometer data [$F^2 > \sigma(F^2)$]. The molecule consists of two almost identical subunits and has 26 chiral C atoms. The central region of the molecule is a macrolidic [Woodward (1957). *Angew. Chem.* **69**, 50–58] sixteen-membered ring with two lactone groups. There are two chains of deoxysaccharides attached to opposite atoms on the macrolidic ring. The molecule has a plate-like conformation with polar and nonpolar sides, which accounts for its action on biological membranes.

Introduction. *Streptomyces albus*, ATCC 21838 (DSM 2566) is able to generate an unusual natural product, salbomycin, which we could not relate to any group of known compounds (Vertesy & Paulus, 1982). *Streptomyces albus* was cultivated aerobically in a complex aqueous medium; salbomycin was then extracted with acetone, purified by chromatography on silica gel and recrystallized. It was not possible to obtain even an approximate structure by spectroscopic methods, and the mass spectrum did not reveal the molecular weight.



(I)

Experimental. Sample recrystallized from methanol, crystal 0·48 × 0·43 × 0·32 mm; molecules are light sensitive in solution, but not in solid state; crystal sealed in Lindemann-glass capillary; 25 reflections with $2\theta > 19{\cdot}6°$ used for cell refinement, 1 standard reflection, variation 2·6%; 3660 of the 4080 unique reflections had $I > \sigma(I)$ and were used for structure analysis; Nicolet $R3$ computer-controlled diffractometer, $2\theta/\theta$ scan, $2\theta_{max} = 110°$, 3° min^{-1}; no corrections for absorption or extinction; $-10 \le h \le 10$, $0 \le k \le 10$, $0 \le l \le 32$. The solution of the phase problem by direct methods proved difficult, although the intensities were collected at low temperature to improve the resolution. After many attempts using a variety of programs the structure was solved by the new random-start multi-solution program *SHELX*84 (G. M. Sheldrick) in an almost routine run. Because there was no prior structural information it was necessary to distinguish between carbon and oxygen atoms. It soon became clear that the molecule consists of two subunits. Although differentiation between O and C was scarcely

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possible in the one half, it was straightforward in the other half. The temperature coefficients, bond lengths and bond angles are all consistent with our assignment. Difference electron density synthesis showed positions of a few hydrogen atoms; in final refinement all hydrogen atoms refined using a model with idealized geometry (C–H 0·96 Å) and temperature factors fixed at 1·2 times the equivalent isotropic values for the C atoms to which they were attached; other atoms refined anisotropically; least-squares refinement on F with 3660 data, 700 parameters, $w = 1/\sigma^2(F)$, $R = 0{\cdot}094$, $R_2(\equiv R_w) = 0{\cdot}053$;* ten largest peaks in final difference electron density synthesis between 0·33 and 0·63 e Å^{-3}; max. $\Delta/\sigma = 0{\cdot}2$; calculations performed with a Nova 3/12 computer and *SHELXTL* (Sheldrick, 1978); scattering factors and f',f'' from *International Tables for X-ray Crystallography* (1974).

Discussion. The atomic parameters are given in Table 1. Fig. 1 shows a drawing of the molecule. It gives the overall conformation and the relative configuration of the 26 chiral C atoms. There is a central macrolidic sixteen-membered ring, which has two lactone groups, each conjugated to two double bonds. The molecule was probably produced by the condensation of two ξ-hydroxycarboxylic acids. The conformations of these two subunits are quite similar. However, the torsion angles about the bonds O(04)–C(23) and O(07)–C(36), which link the six-membered rings, differ by more than 20°, whereas the torsion angles about C(01)–C(15) and C(08)–C(28) (which join the deoxysaccharides to the central ring) are similar to each other (Table 2).

Fig. 2 shows a projection of the molecule parallel to a direction in the macrolidic ring. The conjugated double bonds are *trans* configurated, so that a plate-like molecule results, in which four intramolecular hydrogen bonds are possible [O(09)···O(11) 2·81, O(11)···O(12) 2·70, O(10)···O(15) 2·97, O(15)···O(16) 2·69 Å (e.s.d. 0·01 Å for all O···O distances)]. As a result of this molecular conformation, one side of the molecule is polar and the other non-polar, surely one of the reasons for its biological activity on membranes. It can be seen in Fig. 2, however, that geometrical conditions may also have to be fulfilled for the molecule to be biologically active.

Fig. 3 shows the packing of the molecules and the system of hydrogen bonds. At each end of the molecule, the two free hydroxy groups take part in infinite hydrogen-bonded chains about the twofold screw axes

* Lists of structure factors, anisotropic temperature factors, hydrogen-atom coordinates and bond lengths and angles have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39105 (31 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *The atomic coordinates and the coefficients of the isotropic temperature factors for salbomycin*

The atomic coordinates are given in units of the lattice constants, the isotropic temperature coefficients (in Å^2) were calculated from the anisotropic ones after the last least-squares cycle. The e.s.d.'s are in parentheses.

$$B_{eq} = 8\pi^2(\text{trace } \tilde{\mathbf{U}})/3.$$

	x	y	z	B_{eq}
O(01)	0·1069 (5)	0·7265 (5)	0·5904 (2)	3·0 (2)
O(02)	0·3050 (5)	0·7521 (6)	0·3971 (2)	2·7 (2)
O(03)	0·3181 (5)	0·6650 (5)	0·7374 (2)	2·9 (2)
O(04)	0·3416 (5)	0·6048 (5)	0·8699 (1)	2·7 (2)
O(05)	0·3461 (5)	0·3812 (5)	0·8922 (2)	2·3 (2)
O(06)	0·0855 (5)	0·6489 (5)	0·2609 (1)	2·1 (1)
O(07)	0·0040 (5)	0·6896 (5)	0·1274 (1)	2·3 (2)
O(08)	−0·0333 (5)	0·5101 (5)	0·0803 (2)	3·0 (2)
O(09)	0·2459 (6)	0·5455 (6)	0·5860 (2)	4·8 (2)
O(1)	0·2885 (5)	0·4083 (5)	0·0526 (2)	3·6 (2)
O(10)	0·2104 (6)	0·5453 (6)	0·3991 (2)	4·1 (2)
O(11)	0·1331 (6)	0·4756 (5)	0·6650 (2)	3·2 (2)
O(12)	0·2562 (5)	0·4382 (5)	0·7440 (2)	2·9 (2)
O(13)	0·4416 (5)	0·3339 (6)	0·9843 (2)	3·3 (2)
O(14)	0·4293 (5)	0·6030 (5)	1·0054 (2)	3·5 (2)
O(15)	0·3368 (6)	0·5263 (5)	0·3138 (2)	3·2 (2)
O(16)	0·2267 (5)	0·4831 (5)	0·2336 (2)	3·1 (2)
O(17)	−0·0958 (5)	0·5640 (5)	−0·0115 (2)	3·1 (2)
O(18)	−0·0527 (5)	0·8409 (5)	−0·0017 (2)	2·8 (2)
O(2)	0·0794 (8)	0·2181 (8)	0·0917 (2)	8·7 (3)
C(01)	−0·0074 (8)	0·6468 (8)	0·6037 (2)	3·1 (3)
C(02)	0·2154 (9)	0·6587 (10)	0·5768 (3)	4·1 (3)
C(03)	0·2995 (9)	0·7471 (10)	0·5484 (2)	3·2 (3)
C(04)	0·3880 (8)	0·6931 (10)	0·5228 (2)	3·9 (3)
C(05)	0·4461 (9)	0·7627 (10)	0·4866 (3)	4·0 (3)
C(06)	0·5166 (8)	0·6963 (10)	0·4555 (2)	3·9 (3)
C(07)	0·5460 (8)	0·7515 (9)	0·4132 (2)	3·3 (3)
C(08)	0·4324 (8)	0·7048 (9)	0·3812 (2)	2·7 (3)
C(09)	0·2110 (8)	0·6593 (9)	0·4092 (2)	3·1 (3)
C(10)	0·1164 (9)	0·7280 (9)	0·4367 (3)	3·2 (3)
C(11)	0·0315 (8)	0·6554 (9)	0·4611 (2)	3·3 (3)
C(12)	−0·0391 (8)	0·7100 (9)	0·4984 (3)	3·3 (3)
C(13)	−0·0943 (8)	0·6362 (9)	0·5293 (2)	3·6 (3)
C(14)	−0·1305 (8)	0·6843 (9)	0·5724 (2)	2·7 (3)
C(15)	−0·0246 (8)	0·6655 (8)	0·6523 (2)	2·8 (2)
C(16)	0·1009 (8)	0·6102 (9)	0·6779 (2)	2·9 (3)
C(17)	0·0786 (8)	0·6100 (8)	0·7278 (2)	2·8 (3)
C(18)	0·2183 (9)	0·5732 (8)	0·7532 (2)	3·2 (3)
C(19)	0·4521 (8)	0·6477 (8)	0·7572 (2)	2·8 (2)
C(20)	0·4491 (8)	0·6680 (9)	0·8061 (2)	2·8 (3)
C(21)	0·3491 (8)	0·5733 (8)	0·8250 (2)	2·7 (3)
C(22)	0·2086 (8)	0·5850 (8)	0·8018 (2)	2·7 (3)
C(23)	0·2768 (8)	0·5054 (7)	0·8947 (2)	2·1 (2)
C(24)	0·4855 (8)	0·3846 (8)	0·9086 (2)	2·6 (3)
C(25)	0·5020 (9)	0·4267 (9)	0·9548 (2)	2·8 (3)
C(26)	0·4286 (9)	0·5631 (8)	0·9599 (2)	2·9 (3)
C(27)	0·2840 (8)	0·5557 (8)	0·9407 (2)	2·7 (3)
C(28)	0·4427 (8)	0·7407 (8)	0·3330 (2)	2·7 (3)
C(29)	0·3215 (8)	0·6715 (8)	0·3073 (2)	2·7 (2)
C(30)	0·3194 (8)	0·7002 (9)	0·2583 (2)	2·8 (3)
C(31)	0·1970 (8)	0·6263 (9)	0·2344 (2)	2·9 (3)
C(32)	−0·0462 (8)	0·6003 (9)	0·2436 (2)	2·7 (3)
C(33)	−0·0797 (7)	0·6681 (8)	0·1995 (2)	2·5 (2)
C(34)	0·0300 (7)	0·6308 (9)	0·1694 (2)	2·6 (2)
C(35)	0·1709 (8)	0·6736 (8)	0·1893 (2)	2·8 (3)
C(36)	0·0563 (8)	0·6212 (9)	0·0931 (3)	3·4 (3)
C(37)	−0·1639 (8)	0·5528 (8)	0·0634 (2)	2·7 (2)
C(38)	−0·1537 (8)	0·6359 (8)	0·0230 (3)	3·0 (3)
C(39)	−0·0678 (9)	0·7599 (8)	0·0363 (3)	3·0 (3)
C(40)	0·0780 (8)	0·7159 (8)	0·0548 (2)	2·4 (2)
C(41)	0·6889 (8)	0·7120 (11)	0·3982 (3)	4·6 (3)
C(42)	−0·2642 (8)	0·6244 (10)	0·5861 (3)	4·0 (3)
C(43)	−0·0536 (10)	0·8119 (8)	0·6642 (3)	4·9 (3)
C(44)	−0·0405 (9)	0·5224 (9)	0·7404 (3)	4·8 (3)
C(45)	0·5440 (9)	0·7425 (9)	0·7323 (3)	4·4 (3)
C(46)	0·5929 (8)	0·6572 (8)	0·8281 (3)	3·8 (3)
C(47)	0·6769 (9)	0·5306 (9)	0·8182 (3)	4·6 (3)
C(48)	0·5436 (9)	0·2466 (8)	0·8998 (2)	3·3 (3)
C(49)	0·4329 (9)	0·8950 (8)	0·3267 (3)	4·0 (3)
C(50)	0·4544 (7)	0·6742 (9)	0·2379 (2)	3·5 (3)
C(51)	−0·1461 (8)	0·6220 (9)	0·2785 (2)	3·1 (3)
C(52)	−0·2231 (8)	0·6392 (9)	0·1817 (3)	3·4 (3)
C(53)	−0·2595 (9)	0·4917 (9)	0·1769 (3)	4·3 (3)
C(54)	−0·2547 (9)	0·4262 (8)	0·0558 (3)	3·7 (3)

Table 2. *Torsion angles* (°) *for salbomycin*

The torsion angle $B(1)$–$A(1)$–$A(2)$–$B(2)$ is defined as the angle which the projection of the vector $A(1)\rightarrow B(1)$ onto the plane perpendicular to $A(1)$–$A(2)$ forms with the projection of the vector $A(2)\rightarrow B(2)$ onto the same plane. The e.s.d.'s are given in parentheses.

O(01)–C(01)–C(14)–C(13)	66·4 (8)	C(06)–C(07)–C(08)–O(02)	58·6 (9)	C(29)–C(30)–C(31)–O(16)	−72·0 (8)
O(01)–C(01)–C(14)–C(42)	−171·5 (6)	C(06)–C(07)–C(08)–C(28)	−175·9 (7)	C(29)–C(30)–C(31)–C(35)	167·1 (7)
O(01)–C(01)–C(15)–C(16)	−65·0 (8)	C(07)–C(08)–C(28)–C(29)	175·4 (7)	C(30)–C(31)–C(35)–C(34)	−164·6 (7)
O(01)–C(01)–C(15)–C(43)	60·3 (8)	C(07)–C(08)–C(28)–C(49)	−64·9 (9)	C(31)–O(06)–C(32)–C(33)	−59·1 (8)
O(01)–C(02)–C(03)–C(04)	−162·3 (7)	C(08)–O(02)–C(09)–O(10)	−17·7 (10)	C(31)–O(06)–C(32)–C(51)	174·3 (6)
O(02)–C(08)–C(28)–C(29)	−60·8 (8)	C(08)–O(02)–C(09)–C(10)	161·5 (6)	C(32)–O(06)–C(31)–O(16)	−69·2 (7)
O(02)–C(08)–C(28)–C(49)	58·9 (8)	C(08)–C(28)–C(29)–O(15)	−60·8 (7)	C(32)–O(06)–C(31)–C(30)	174·4 (6)
O(02)–C(09)–C(10)–C(11)	−165·3 (7)	C(08)–C(28)–C(29)–C(30)	179·7 (7)	C(32)–O(06)–C(31)–C(35)	51·8 (9)
O(03)–C(18)–C(22)–C(21)	−52·3 (9)	C(09)–O(02)–C(08)–C(07)	−116·1 (7)	C(32)–C(33)–C(34)–O(07)	179·3 (6)
O(03)–C(19)–C(20)–C(21)	57·2 (8)	C(09)–O(02)–C(08)–C(28)	113·7 (7)	C(32)–C(33)–C(34)–C(35)	−57·6 (8)
O(03)–C(19)–C(20)–C(46)	−177·1 (6)	C(09)–C(10)–C(11)–C(12)	162·3 (7)	C(32)–C(33)–C(52)–C(53)	−55·4 (9)
O(04)–C(21)–C(22)–C(18)	171·1 (6)	C(10)–C(11)–C(12)–C(13)	−162·3 (8)	C(33)–C(34)–C(35)–C(31)	51·5 (9)
O(04)–C(23)–C(27)–C(26)	−66·1 (8)	C(11)–C(12)–C(13)–C(14)	161·9 (7)	C(34)–O(07)–C(36)–O(08)	80·4 (7)
O(05)–C(23)–C(27)–C(26)	54·0 (8)	C(12)–C(13)–C(14)–C(01)	−96·8 (9)	C(34)–O(07)–C(36)–C(40)	−155·9 (6)
O(05)–C(24)–C(25)–O(13)	64·7 (9)	C(12)–C(13)–C(14)–C(42)	140·6 (8)	C(34)–C(33)–C(52)–C(53)	68·3 (9)
O(05)–C(24)–C(25)–C(26)	−54·2 (9)	C(14)–C(01)–C(15)–C(16)	174·2 (7)	C(36)–O(07)–C(34)–C(33)	−152·5 (6)
O(06)–C(31)–C(35)–C(34)	−46·9 (9)	C(14)–C(01)–C(15)–C(43)	−60·5 (9)	C(36)–O(07)–C(34)–C(35)	85·3 (8)
O(06)–C(32)–C(33)–C(34)	61·2 (8)	C(15)–C(01)–C(14)–C(13)	−171·0 (7)	C(36)–O(08)–C(37)–C(38)	61·5 (8)
O(06)–C(32)–C(33)–C(52)	−172·0 (6)	C(15)–C(01)–C(14)–C(42)	−48·9 (10)	C(36)–O(08)–C(37)–C(54)	−173·8 (6)
O(07)–C(34)–C(35)–C(31)	174·3 (6)	C(15)–C(16)–C(17)–C(18)	−171·4 (6)	C(37)–O(08)–C(36)–O(07)	65·5 (7)
O(07)–C(36)–C(40)–C(39)	−68·6 (8)	C(15)–C(16)–C(17)–C(44)	61·8 (9)	C(37)–O(08)–C(36)–C(40)	−57·8 (8)
O(08)–C(36)–C(40)–C(39)	54·6 (8)	C(16)–C(17)–C(18)–O(03)	53·1 (8)	C(37)–C(38)–C(39)–O(18)	178·7 (6)
O(08)–C(37)–C(38)–O(17)	62·0 (8)	C(16)–C(17)–C(18)–O(12)	−66·2 (8)	C(37)–C(38)–C(39)–C(40)	59·4 (8)
O(08)–C(37)–C(38)–C(39)	−61·1 (8)	C(16)–C(17)–C(18)–C(22)	174·0 (7)	C(38)–C(39)–C(40)–C(36)	−57·2 (8)
O(09)–C(02)–C(03)–C(04)	19·1 (12)	C(17)–C(18)–C(22)–C(21)	−170·0 (7)	C(41)–C(07)–C(08)–O(02)	−177·3 (7)
O(10)–C(09)–C(10)–C(11)	13·8 (12)	C(18)–O(03)–C(19)–C(20)	−59·9 (8)	C(41)–C(07)–C(08)–C(28)	−51·8 (10)
O(11)–C(16)–C(17)–C(18)	65·1 (8)	C(18)–O(03)–C(19)–C(45)	173·6 (6)	C(43)–C(15)–C(16)–O(11)	−176·7 (6)
O(11)–C(16)–C(17)–C(44)	−61·7 (8)	C(19)–O(03)–C(18)–O(12)	−61·6 (7)	C(43)–C(15)–C(16)–C(17)	62·1 (9)
O(12)–C(18)–C(22)–C(21)	68·6 (8)	C(19)–O(03)–C(18)–C(17)	179·4 (6)	C(44)–C(17)–C(18)–O(03)	−179·9 (6)
O(13)–C(25)–C(26)–O(14)	51·7 (8)	C(19)–O(03)–C(18)–C(22)	57·5 (8)	C(44)–C(17)–C(18)–O(12)	60·8 (8)
O(13)–C(25)–C(26)–C(27)	−71·2 (7)	C(19)–C(20)–C(21)–O(04)	−174·9 (6)	C(44)–C(17)–C(18)–C(22)	−58·9 (9)
O(14)–C(26)–C(27)–C(23)	−175·9 (6)	C(19)–C(20)–C(21)–C(22)	−53·6 (9)	C(45)–C(19)–C(20)–C(21)	176·8 (7)
O(15)–C(29)–C(30)–C(31)	60·1 (8)	C(19)–C(20)–C(46)–C(47)	−52·2 (10)	C(45)–C(19)–C(20)–C(46)	−57·6 (9)
O(15)–C(29)–C(30)–C(50)	−67·9 (8)	C(20)–C(21)–C(22)–C(18)	51·8 (9)	C(46)–C(20)–C(21)–O(04)	59·8 (8)
O(16)–C(31)–C(35)–C(34)	74·4 (8)	C(21)–O(04)–C(23)–O(05)	58·8 (7)	C(46)–C(20)–C(21)–C(22)	−178·9 (6)
O(17)–C(38)–C(39)–O(18)	55·5 (8)	C(21)–O(04)–C(23)–C(27)	178·2 (6)	C(48)–C(24)–C(25)–O(13)	−56·6 (9)
O(17)–C(38)–C(39)–C(40)	−63·8 (8)	C(21)–C(20)–C(46)–C(47)	72·1 (9)	C(48)–C(24)–C(25)–C(26)	−175·5 (7)
O(18)–C(39)–C(40)–C(36)	−175·8 (6)	C(23)–O(04)–C(21)–C(20)	−165·9 (6)	C(49)–C(28)–C(29)–O(15)	179·1 (6)
C(01)–O(01)–C(02)–O(09)	−23·4 (11)	C(23)–O(04)–C(21)–C(22)	72·8 (8)	C(49)–C(28)–C(29)–C(30)	59·6 (8)
C(01)–O(01)–C(02)–C(03)	158·0 (6)	C(23)–O(05)–C(24)–C(25)	58·6 (8)	C(50)–C(30)–C(31)–O(06)	173·1 (6)
C(01)–C(15)–C(16)–O(11)	−51·1 (8)	C(23)–O(05)–C(24)–C(48)	−175·7 (6)	C(50)–C(30)–C(31)–O(16)	56·7 (8)
C(01)–C(15)–C(16)–C(17)	−172·4 (7)	C(24)–O(05)–C(23)–O(04)	61·1 (7)	C(50)–C(30)–C(31)–C(35)	−64·2 (9)
C(02)–O(01)–C(01)–C(14)	−118·2 (7)	C(24)–O(05)–C(23)–C(27)	−55·6 (8)	C(51)–C(32)–C(33)–C(34)	−178·5 (7)
C(02)–O(01)–C(01)–C(15)	114·1 (7)	C(24)–C(25)–C(26)–O(14)	174·2 (6)	C(51)–C(32)–C(33)–C(52)	−51·7 (9)
C(02)–C(03)–C(04)–C(05)	163·1 (7)	C(24)–C(25)–C(26)–C(27)	51·2 (8)	C(52)–C(33)–C(34)–O(07)	52·8 (9)
C(03)–C(04)–C(05)–C(06)	−166·9 (8)	C(25)–C(26)–C(27)–C(23)	−52·9 (8)	C(52)–C(33)–C(34)–C(35)	176·0 (7)
C(04)–C(05)–C(06)–C(07)	163·2 (8)	C(28)–C(29)–C(30)–C(31)	179·1 (6)	C(54)–C(37)–C(38)–O(17)	−59·9 (8)
C(05)–C(06)–C(07)–C(08)	−94·4 (10)	C(28)–C(29)–C(30)–C(50)	51·2 (9)	C(54)–C(37)–C(38)–C(39)	177·1 (6)
C(05)–C(06)–C(07)–C(41)	142·3 (9)	C(29)–C(30)–C(31)–O(06)	44·4 (8)		

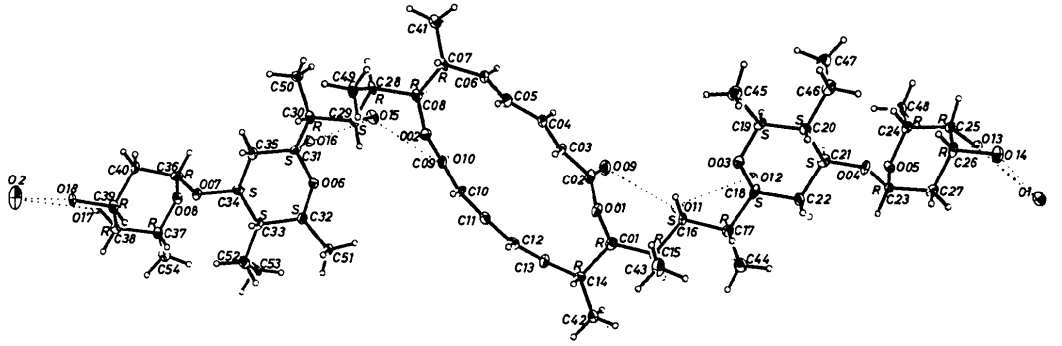

Fig. 1. Molecular structure of salbomycin, showing 30% probability thermal ellipsoids for the non-hydrogen atoms and the atom-numbering scheme.

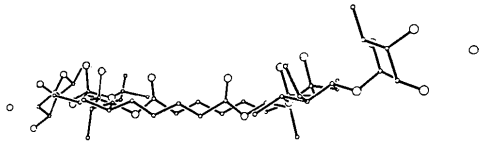

Fig. 2. Projection of the molecule, viewed parallel to a direction in the macrolidic ring.

[O(13)···O(14^{ii}) 2·65, O(17)···O(18^{i}) 2·69 Å].* Each pair of hydroxy groups also makes an approximately equilateral triangle with a water molecule [O(13)···O(1^{ii}) 2·74, O(14)···O(1^{iii}) 2·83; O(17)···O(2^{i}) 2·93,

* Symmetry operations (i) $-x$, $0{\cdot}5+y$, $-z$; (ii) $1-x$, $0{\cdot}5+y$, $2-z$; (iii) x, y, $1+z$.

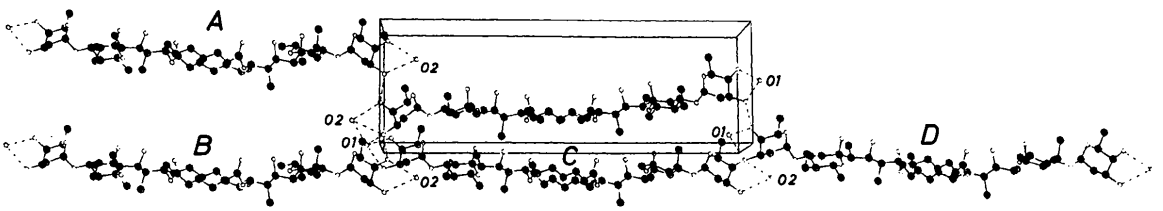

Fig. 3. The environment of one molecule, viewed parallel to a direction in the macrolidic ring.

O(18)···O(2^{i}) 3·04 Å], suggesting disordered or bifurcated hydrogen bonds involving the remaining hydroxyl protons. Each water molecule is then in a position to make two further hydrogen bonds [O(1^{i})···O(18) 2·81, O(1)···O(2) 3·08, O(2)···O(08) 3·15 Å].

Streptomyces albus ATCC 21838 is also able to generate polyether antibiotics of the salinomycin group (Miyazaki, Shibuya, Sugawara, Kawaguchi, Hirose, Nagatsu & Esumi, 1974). The structural formulae indicate that the biosynthesis of the two compounds follows similar paths. In the case of salbomycin the terminal saccharides are 2-deoxyfucose, a component of the antibiotic olivomycin (Berlin, Esipov, Kiseleva & Kolosov, 1967).

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Structure of a Favorskii Substitution Product, 3β-Acetoxy-17β-hydroxy-18-nor-5α,17α-pregnan-20-one,* $C_{22}H_{34}O_4$†

BY C. P. HUBER AND F. R. AHMED

Division of Biological Sciences, National Research Council of Canada, Ottawa, Canada K1A 0R6

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Abstract. $M_r = 362·5$, monoclinic, $C2$, $a = 14·746$ (4), $b = 7·483$ (4), $c = 36·916$ (20) Å, $\beta = 97·40$ (4)°, $V = 4039·5$ Å^3, $Z = 8$ (two molecules per asymmetric unit), $D_m = 1·188$ (4), $D_x = 1·192$ Mg m^{-3}, Cu $K\alpha_1$, $\lambda = 1·54056$ Å, $\mu = 0·60$ mm^{-1}, $F(000) = 1584$, $T = 293$ K, final $R = 0·049$ for 3704 observed reflections. The hydroxyl group at C(17) is β, *cis* to the C(19) methyl group. Rings *A*, *B* and *C* show essentially identical chair conformations in the two molecules, while ring *D*, here in the uncommon C(14)-envelope form, shows some small conformational differences, which may be related to the intermolecular hydrogen-bonding pattern.

Introduction. The title compound was obtained as a substitution product in a Favorskii rearrangement reaction of 3β-acetoxy-17-bromo-18-nor-5α-pregnan-20-one. Such substitution products from α-halogenated ketones are considered to be formed *via* epoxy ether intermediates, and subsequent hydrolysis of the epoxy ether (Engel, Lachance, Capitaine, Zee, Mukherjee & Mérand, 1983). The usual opening of the epoxy ring would result in an overall inversion of configuration at C(17), and the evidence suggested that it had done so in this case (Engel *et al.*, 1983), but a weakly positive Cotton effect of the title compound would have been compatible with a 17α-hydroxy configuration. The crystal structure was examined in order to establish the stereochemistry unambiguously, and confirmed that the hydroxyl group at C(17) was indeed in the expected β configuration.

* IUPAC nomenclature: 20-oxo-18-nor-5α,17α-pregnane-3β,17β-diol 3-monoacetate.

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