Table 1. *Atomic coordinates and equivalent isotropic thermal parameters* (Å^2) *of the non-*H *atoms with e.s.d.'s in parentheses*

$$B_{eq} = \tfrac{4}{3}\Sigma_i\Sigma_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
N(1)	0.54041 (15)	0.38421 (12)	0.0047 (2)	1.97 (3)
C(2)	0.4251 (2)	0.42902 (15)	0.1069 (2)	2.37 (4)
C(3)	0.6452 (2)	0.47274 (15)	0.0251 (2)	2.42 (4)
C(4)	0.6125 (2)	0.28927 (16)	0.0806 (2)	2.64 (4)
C(5)	0.5229 (2)	0.18449 (16)	0.0871 (2)	2.91 (5)
O(6)	0.41560 (14)	0.18422 (11)	0.2090 (2)	2.95 (4)

Table 2. *Intramolecular interatomic distances* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

N(1)—C(2)	1.471 (2)	N(1)—C(3)	1.471 (2)
N(1)—C(4)	1.471 (2)	C(4)—C(5)	1.520 (3)
C(5)—O(6)	1.419 (3)	C(2)—C(3')	1.514 (2)

C(2)—N(1)—C(3)	108.2 (1)	C(2)—N(1)—C(4)	112.2 (1)
C(3)—N(1)—C(4)	109.7 (1)	N(1)—C(4)—C(5)	114.6 (2)
C(4)—C(5)—O(6)	114.5 (2)	N(1)—C(2)—C(3')	110.5 (2)
N(1)—C(3)—C(2')	111.0 (2)		

$3\sigma(F_o)$ and 91 variables. $(\Delta/\sigma)_{max} = 0.03$. Final difference map contained no peak higher than 0.3 e Å^{-3}. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV). All the calculations were performed on an NEC ACOS-930 computer of the Protein Engineering Research Center, Institute for Protein Research, Osaka University.

The numbering scheme and the thermal ellipsoids of all the atoms are illustrated in Fig. 1. Positional parameters are given in Table 1.* Bond lengths and angles are given in Table 2.

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* Lists of structure amplitudes, anisotropic thermal parameters for non-H atoms, and positional parameters and isotropic thermal parameters for all H atoms have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55003 (7 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Related literature. Gas electron-diffraction studies: Davis & Hassel (1963); Yokozeki & Kuchitsu (1971). IR spectra studies: Cook, Jones, Katritzky, Manas, Richards, Sparrow & Trepanier (1973); Imbach, Jones, Katritzky & Wyatt (1967); Baldock & Katritzky (1968); Bishop, Sutton, Dineen, Jones, Katritzky & Wyatt (1967). Related compounds: Okamoto, Sekido, Itoh, Noguchi & Hirokawa (1979); Okamoto, Sekido, Ono, Noguchi & Hirokawa (1982); Sekido, Okamoto & Hirokawa (1985).

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Structure of Concanamycin A Pentahydrate

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Abstract. Concanamycin A was obtained from the culture broth of *Streptomyces diastatochromogenese* PA-48098. Three crystal forms of concanamycin A were obtained, (I*a*) from methanol–water, (II) from ethanol–water and (I) on drying (I*a*). (I): $C_{46}H_{75}NO_{14}.5H_2O$, $M_r = 956.17$, monoclinic, $P2_1$, a

$= 24.376$ (3), $b = 10.816$ (2), $c = 9.983$ (1) Å, $\beta = 92.71$ (1)°, $V = 2629.2$ (7) Å^3, $Z = 2$, $D_x = 1.208$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.54178 Å, $\mu = 0.78$ mm^{-1}, $F(000) = 1040$, $T = 295$ K, $R = 0.055$ for 3208 observed reflections. The crystal structure contains five water molecules, one of which has an occupancy of 0.2. There is one intramolecular hydrogen bond, O22···HO31 [2.736 (6) Å], and two intermolecular hydrogen bonds, O46···HO43 $(2 - x, \frac{1}{2} + y, 2 - z)$ [2.807 (7) Å] and O53···HN47$(-1 - x, \frac{1}{2} + y, -1 - z)$ [2.922 (9) Å].

Experimental. Rigaku AFC-5R diffractometer, graphite-monochromatized Cu $K\alpha$ radiation. Structures obtained by $MULTAN$87 (Debaerdemaeker, Germain, Main, Tate & Woolfson, 1987). Atomic scattering factors calculated by $\Sigma a_i \exp(-b_i \lambda^{-2} \times \sin^2\theta)] + c$ $(i = 1,...,4)$ (*International Tables for X-ray Crystallography*, 1974, Vol. IV). Calculations performed on VAX station 3100 computer at Shionogi Research Laboratories.

(I)
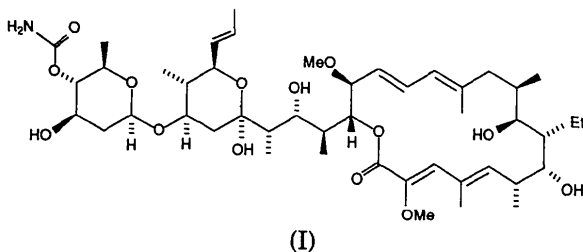
Colorless plate crystals of (Ia) were grown from methanol–water. The crystals were unstable in air when separated from the mother liquor, so a crystal was sealed in a glass capillary. However, intensities of X-ray diffractions from the crystal were very weak and the crystal structure could not been solved.

The crystal of (I) was obtained by good fortune when the mother liquor sealed with (Ia) was lost through an accidental leak. The crystal of dimensions 0.4 × 0.2 × 0.1 mm was resealed. Cell dimensions determined from 2θ angles for 25 reflections in the range $22 < 2\theta < 46°$. Intensities measured up to $\theta = 65°$ with h $-27/27$, k $-12/0$ and l $-12/0$; ω–2θ scans, ω-scan width $(1.2 + 0.2\tan\theta)°$. Three standard reflections monitored every 100 measurements showed 3% decay, intensities corrected. 4697 unique reflections measured, 3208 intensities observed [those with $F_o \leq 3\sigma(F_o)$ and two very strong reflections rejected], no absorption corrections. H atoms except those attached to O22, the amino group and the water molecules were located on a difference density map. H atoms of the amino group were calculated and placed at their ideal positions. All atoms refined with block-diagonal least-squares method, with anisotropic temperature factors for the non-H atoms

Table 1. *Atomic coordinates and equivalent isotropic temperature factors* (Å^2)

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

	x	y	z	B_{eq}
C1	0.4703 (2)	0.300	0.9481 (5)	2.8 (1)
C2	0.4216 (2)	0.2424 (6)	1.0165 (5)	3.5 (1)
C3	0.3680 (2)	0.3071 (6)	0.9787 (6)	3.8 (1)
C4	0.3214 (2)	0.2503 (6)	0.9498 (5)	3.6 (1)
C5	0.2694 (2)	0.3102 (6)	0.9193 (5)	3.4 (1)
C6	0.2197 (2)	0.2631 (6)	0.9070 (6)	4.4 (2)
C7	0.1693 (2)	0.3396 (7)	0.8866 (5)	4.3 (2)
C8	0.1307 (2)	0.3053 (6)	0.7618 (6)	4.2 (2)
C9	0.1257 (2)	0.4183 (3)	0.6687 (6)	3.8 (1)
C10	0.1784 (2)	0.4523 (6)	0.5974 (5)	3.9 (2)
C11	0.1856 (2)	0.3799 (7)	0.4659 (6)	4.6 (2)
C12	0.2401 (2)	0.4047 (8)	0.4014 (5)	5.3 (2)
C13	0.2892 (2)	0.3834 (6)	0.4965 (5)	4.1 (2)
C14	0.3380 (2)	0.4362 (7)	0.4920 (5)	4.3 (2)
C15	0.3791 (2)	0.4081 (6)	0.6011 (5)	3.6 (1)
C16	0.4283 (2)	0.4560 (6)	0.6288 (5)	3.8 (2)
C17	0.4604 (2)	0.4323 (6)	0.7558 (6)	3.5 (1)
O18	0.4505 (1)	0.3201 (4)	0.8078 (3)	3.5 (1)
C19	0.5220 (2)	0.2193 (5)	0.9532 (5)	3.1 (1)
C20	0.5190 (2)	0.1165 (6)	0.8473 (6)	3.9 (2)
C21	0.5737 (2)	0.2988 (6)	0.9427 (5)	3.2 (1)
O22	0.5764 (1)	0.3931 (4)	1.0457 (4)	3.8 (1)
C23	0.6284 (2)	0.2244 (5)	0.9488 (5)	2.9 (1)
C24	0.6417 (2)	0.1697 (6)	1.0881 (6)	4.3 (2)
C25	0.6754 (2)	0.3061 (5)	0.9008 (5)	3.0 (1)
O26	0.6593 (1)	0.3371 (4)	0.7659 (3)	3.4 (1)
C27	0.6976 (2)	0.4100 (6)	0.6960 (6)	3.8 (1)
C28	0.7537 (2)	0.3487 (6)	0.6928 (5)	3.9 (2)
C29	0.7737 (2)	0.3095 (6)	0.8329 (6)	3.7 (1)
C30	0.7304 (2)	0.2374 (6)	0.9026 (5)	3.6 (1)
O31	0.6837 (1)	0.4138 (4)	0.9799 (4)	3.8 (1)
C32	0.6715 (2)	0.4276 (7)	0.5581 (6)	4.5 (2)
C33	0.6663 (3)	0.5318 (8)	0.4932 (6)	5.3 (2)
C34	0.6427 (4)	0.5465 (10)	0.3516 (8)	7.5 (3)
C35	0.7961 (3)	0.4309 (9)	0.6273 (8)	6.8 (3)
O36	0.8226 (1)	0.2378 (4)	0.8147 (3)	3.9 (1)
C37	0.8509 (2)	0.1977 (6)	0.9314 (6)	3.6 (1)
C38	0.9014 (2)	0.1286 (6)	0.8886 (6)	4.0 (2)
C39	0.9390 (2)	0.0966 (6)	1.0077 (6)	3.9 (2)
C40	0.9520 (2)	0.2133 (6)	1.0894 (6)	3.8 (1)
C41	0.8978 (2)	0.2727 (6)	1.1297 (6)	4.3 (2)
O42	0.8673 (1)	0.3047 (4)	1.0076 (4)	3.7 (1)
O43	0.9896 (1)	0.0451 (4)	0.9672 (4)	4.6 (1)
O44	0.9830 (2)	0.1760 (4)	1.2099 (4)	4.6 (1)
C45	1.0226 (2)	0.2521 (7)	1.2583 (7)	5.3 (2)
O46	1.0371 (2)	0.3449 (5)	1.2025 (5)	6.7 (2)
N47	1.0438 (3)	0.2135 (6)	1.3768 (6)	6.4 (2)
C48	0.9044 (3)	0.3903 (7)	1.2125 (7)	5.1 (2)
O49	0.4354 (1)	0.2599 (4)	1.1567 (3)	4.1 (1)
C50	0.4016 (3)	0.1899 (8)	1.2410 (6)	5.6 (2)
C51	0.2097 (3)	0.1263 (8)	0.9227 (12)	9.3 (4)
C52	0.0754 (3)	0.2610 (7)	0.8089 (7)	5.6 (2)
O53	0.0823 (1)	0.4034 (5)	0.5671 (4)	5.0 (1)
C54	0.1793 (3)	0.5939 (8)	0.5713 (8)	6.3 (2)
C55	0.2217 (4)	0.6605 (10)	0.6533 (11)	8.7 (3)
O56	0.1818 (2)	0.2499 (5)	0.4943 (5)	6.3 (1)
C57	0.2434 (3)	0.3320 (12)	0.2707 (7)	8.6 (3)
C58	0.3521 (3)	0.5274 (10)	0.3851 (7)	6.9 (3)
O59	0.4493 (2)	0.5536 (5)	0.5558 (4)	5.3 (1)
C60	0.5010 (4)	0.5288 (10)	0.5033 (9)	7.0 (3)
O61	0.4926 (2)	0.5060 (4)	0.8041 (4)	4.3 (1)
Ow1	0.5398 (2)	0.2937 (5)	1.2906 (4)	5.7 (1)
Ow2	0.9243 (2)	0.4769 (6)	0.8384 (5)	7.3 (2)
Ow3	0.9677 (2)	0.3861 (9)	0.6052 (6)	10.0 (3)
Ow4	0.9680 (3)	0.0953 (8)	0.5905 (7)	10.8 (3)
Ow5*	0.141 (1)	0.193 (3)	0.215 (3)	8.5 (7)

* Occupancy factor 0.2.

except Ow5, which was refined isotropically; the temperature factor for each H atom was set equal to B_{eq} of the bonded atom; 664 parameters refined. $\Sigma(w|\Delta F|^2)$ minimized, $w = 1/[\sigma^2(F_o) + 0.00188|F_o|^2]$, $w = 0$ for 36 reflections with $w^{1/2}|\Delta F| > 3$. Final $R = 0.055$, $wR = 0.065$, $S = 1.135$. Highest and lowest peaks in the final difference map were 0.2 and -0.2 e Å^{-3}. Max. Δ/σ in the final cycle 0.1.
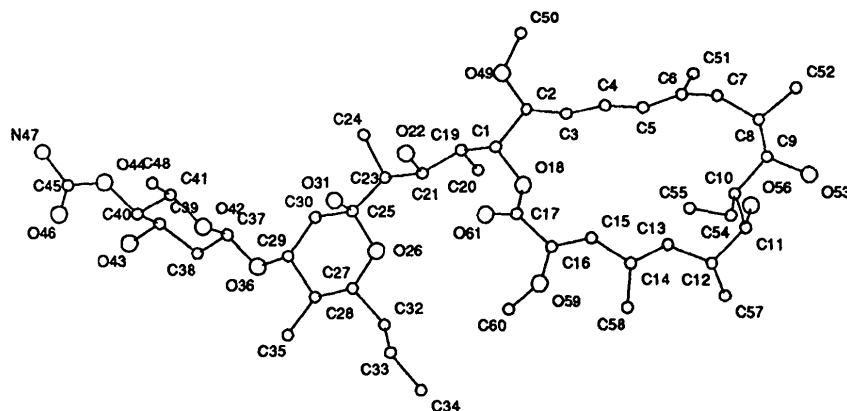
Fig. 1. Perspective view of (I) drawn by *PLUTO* (Motherwell & Clegg, 1978).

The final atomic coordinates and equivalent isotropic temperature factors are given in Table 1.* A perspective view of the molecule with atom labelling is presented in Fig. 1.

The other crystal data are as follows. For (I*a*): monoclinic, *C*2, *a* = 61.384 (11), *b* = 10.913 (2), *c* = 9.972 (2) Å, β = 93.94 (2)°, *V* = 6664 (2) Å³, *Z* = 4; for (II): orthorhombic, *P*2₁2₁2₁, *a* = 11.179 (6), *b* = 53.567 (7), *c* = 9.646 (1) Å, *V* = 5776 (3) Å³, *Z* = 4.

Related literature. Concanamycin A has also been produced from *Streptomyces diastatochromogenes* S45 by Kinashi, Someno & Sakaguchi (1980). An antifungal antibiotic A661-I, isolated by Shoji,

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* Lists of H-atom coordinates, anisotropic temperature factors for the non-H atoms, bond lengths, bond angles and structure factors for (I) have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54957 (36 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: AS0564]

Wakisaka, Mayama & Watanabe (1974), is a mixture (1:1) of concanamycins A and B. The crystal structure of concanamycin A diacetate was analyzed because suitable crystals of concanamycin A had not been obtained (Westley, Liu, Sello, Evans, Troupe, Blount, Chiu, Todaro & Miller, 1984).

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The Structure of a Trisubstituted 3*H*-1,2-Dithiole

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Abstract. *N*-Phenyl-5-phenylamino-3-phenylimino-3*H*-1,2-dithiole-4-carbothioamide, C₂₂H₁₇N₃S₃, *M*ᵣ = 419.59, monoclinic, *P*2₁/*n*, *a* = 12.8198 (9), *b* = 6.9843 (8), *c* = 23.0717 (13) Å, β = 102.981 (5)°, *V* = 2013.0 (3) Å³, *Z* = 4, *D*ₓ = 1.390 Mg m⁻³, Mo *K*α, λ = 0.71073 Å, μ = 36.67 mm⁻¹, *T* = 291 K, *R* = 0.060, *wR* = 0.060 for 2323 unique reflections with *I* > 2σ(*I*). The phenylthiocarbamido part of the 1,2-dithiole ring is significantly conjugated and the conjugated system includes the N(1) and N(2) atoms of